

# THE REGULARIZATION THEORY OF THE KRYLOV ITERATIVE SOLVERS LSQR, CGLS, LSMR AND CGME FOR LINEAR DISCRETE ILL-POSED PROBLEMS\*

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**Abstract.** For the large-scale linear discrete ill-posed problem  $\min \|Ax - b\|$  or  $Ax = b$  with  $b$  contaminated by a white noise, the Lanczos bidiagonalization based Krylov solver LSQR and its mathematically equivalent CGLS are most commonly used. They have intrinsic regularizing effects, where the number  $k$  of iterations plays the role of regularization parameter. However, there has been no answer to the long-standing fundamental concern: *for which kinds of problems LSQR and CGLS can find best possible regularized solutions?* The concern was actually expressed foresightedly by Björck and Eldén in 1979. Here a best possible regularized solution means that it is at least as accurate as the best regularized solution obtained by the truncated singular value decomposition (TSVD) method, which and the best possible solution by standard-form Tikhonov regularization are both of the same order of the worst-case error and cannot be improved under the assumption that the solution to an underlying linear compact operator equation is continuous or its derivative squares integrable. In this paper we make a detailed analysis on the regularization of LSQR for severely, moderately and mildly ill-posed problems. We first consider the case that the singular values of  $A$  are simple. We establish accurate  $\sin \Theta$  theorems for the 2-norm distance between the underlying  $k$ -dimensional Krylov subspace and the  $k$ -dimensional dominant right singular subspace of  $A$ . Based on them and some follow-up results, for the first two kinds of problems, we prove that LSQR finds a best possible regularized solution at semi-convergence occurring at iteration  $k_0$  and the following results hold for  $k = 1, 2, \dots, k_0$ : (i) the  $k$ -step Lanczos bidiagonalization always generates a near best rank  $k$  approximation to  $A$ ; (ii) the  $k$  Ritz values always approximate the first  $k$  large singular values in natural order; (iii) the  $k$ -step LSQR always captures the  $k$  dominant SVD components of  $A$ . However, for the third kind of problem, we prove that LSQR cannot find a best possible regularized solution generally. We derive accurate estimates for the diagonals and subdiagonals of the bidiagonal matrices generated by Lanczos bidiagonalization, which can be used to decide if LSQR finds a best possible regularized solution at semi-convergence. We also analyze the regularization of the other two Krylov solvers LSMR and CGME that are MINRES and the CG method applied to  $A^T Ax = A^T b$  and  $\min \|AA^T y - b\|$  with  $x = A^T y$ , respectively, proving that the regularizing effects of LSMR are similar to LSQR for each kind of problem and both are superior to CGME. We extend all the results to the case that  $A$  has multiple singular values. Numerical experiments confirm our theory on LSQR.

**Key words.** Discrete ill-posed, full or partial regularization, best or near best rank  $k$  approximation, TSVD solution, semi-convergence, Lanczos bidiagonalization, LSQR, CGLS, LSMR, CGME

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**1. Introduction and Preliminaries.** Consider the linear discrete ill-posed problem

$$(1.1) \quad \min_{x \in \mathbb{R}^n} \|Ax - b\| \quad \text{or} \quad Ax = b, \quad A \in \mathbb{R}^{m \times n}, \quad b \in \mathbb{R}^m,$$

where the norm  $\|\cdot\|$  is the 2-norm of a vector or matrix, and  $A$  is extremely ill conditioned with its singular values decaying to zero without a noticeable gap. (1.1) mainly arises from the discretization of the first kind Fredholm integral equation

$$(1.2) \quad Kx = (Kx)(t) = \int_{\Omega} k(s, t)x(t)dt = g(s) = g, \quad s \in \Omega \subset \mathbb{R}^q,$$

where the kernel  $k(s, t) \in L^2(\Omega \times \Omega)$  and  $g(s)$  are known functions, while  $x(t)$  is the unknown function to be sought. If  $k(s, t)$  is non-degenerate and  $g(s)$  satisfies

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the Picard condition, there exists the unique squares integrable solution  $x(t)$ ; see [27, 53, 56, 81, 89]. Here for brevity we assume that  $s$  and  $t$  belong to the same set  $\Omega \subset \mathbb{R}^q$  with  $q \geq 1$ . Applications include image deblurring, signal processing, geophysics, computerized tomography, heat propagation, biomedical and optical imaging, ground-water modeling, and many others; see, e.g., [1, 26, 27, 56, 66, 75, 76, 81, 89, 90, 119]. The theory and numerical treatments of integral equations can be found in [81, 82]. The right-hand side  $b = \hat{b} + e$  is noisy and assumed to be contaminated by a white noise  $e$ , caused by measurement, modeling or discretization errors, where  $\hat{b}$  is noise-free and  $\|e\| < \|\hat{b}\|$ . Because of the presence of noise  $e$  and the extreme ill-conditioning of  $A$ , the naive solution  $x_{naive} = A^\dagger b$  of (1.1) bears no relation to the true solution  $x_{true} = A^\dagger \hat{b}$ , where  $\dagger$  denotes the Moore-Penrose inverse of a matrix. Therefore, one has to use regularization to extract a best possible approximation to  $x_{true}$ .

The most common regularization, in its simplest form, is the direct standard-form Tikhonov regularization

$$(1.3) \quad \min_{x \in \mathbb{R}^n} \|Ax - b\|^2 + \lambda^2 \|x\|^2$$

with  $\lambda > 0$  the regularization parameter [101, 111, 112]. The solutions to (1.1) and (1.3) can be fully analyzed by the singular value decomposition (SVD) of  $A$ . Let

$$(1.4) \quad A = U \begin{pmatrix} \Sigma \\ \mathbf{0} \end{pmatrix} V^T$$

be the SVD of  $A$ , where  $U = (u_1, u_2, \dots, u_m) \in \mathbb{R}^{m \times m}$  and  $V = (v_1, v_2, \dots, v_n) \in \mathbb{R}^{n \times n}$  are orthogonal,  $\Sigma = \text{diag}(\sigma_1, \sigma_2, \dots, \sigma_n) \in \mathbb{R}^{n \times n}$  with the singular values  $\sigma_1 > \sigma_2 > \dots > \sigma_n > 0$  assumed to be simple throughout the paper except Section 7, and the superscript  $T$  denotes the transpose of a matrix or vector. Then

$$(1.5) \quad x_{naive} = \sum_{i=1}^n \frac{u_i^T b}{\sigma_i} v_i = \sum_{i=1}^n \frac{u_i^T \hat{b}}{\sigma_i} v_i + \sum_{i=1}^n \frac{u_i^T e}{\sigma_i} v_i = x_{true} + \sum_{i=1}^n \frac{u_i^T e}{\sigma_i} v_i$$

$$\text{with } \|x_{true}\| = \|A^\dagger \hat{b}\| = \left( \sum_{k=1}^n \frac{|u_k^T \hat{b}|^2}{\sigma_k^2} \right)^{1/2}.$$

Throughout the paper, we always assume that  $\hat{b}$  satisfies the discrete Picard condition  $\|A^\dagger \hat{b}\| \leq C$  with some constant  $C$  for  $n$  arbitrarily large [1, 33, 50, 51, 53, 56, 76]. It is an analog of the Picard condition in the finite dimensional case; see, e.g., [50], [53, p.9], [56, p.12] and [76, p.63]. This condition means that, on average, the Fourier coefficients  $|u_i^T \hat{b}|$  decay faster than  $\sigma_i$  and enables regularization to compute useful approximations to  $x_{true}$ , which results in the following popular model that is used throughout Hansen's books [53, 56] and the current paper:

$$(1.6) \quad |u_i^T \hat{b}| = \sigma_i^{1+\beta}, \quad \beta > 0, \quad i = 1, 2, \dots, n,$$

where  $\beta$  is a model parameter that controls the decay rates of  $|u_i^T \hat{b}|$ . Hansen [56, p.68] points out, "while this is a crude model, it reflects the overall behavior often found in real problems." One precise definition of the discrete Picard condition is  $|u_i^T \hat{b}| = \tau_i \sigma_i^{1+\zeta_i}$  with certain constants  $\tau_i \geq 0$ ,  $\zeta_i > 0$ ,  $i = 1, 2, \dots, n$ . We remark that once the  $\tau_i > 0$  and  $\zeta_i$  do not differ greatly, such discrete Picard condition does not affect our claims, rather it complicates derivations and forms of the results.

The white noise  $e$  has a number of attractive properties which play a critical role in the regularization analysis: Its covariance matrix is  $\eta^2 I$ , the expected values

$\mathcal{E}(\|e\|^2) = m\eta^2$  and  $\mathcal{E}(|u_i^T e|) = \eta$ ,  $i = 1, 2, \dots, n$ , and  $\|e\| \approx \sqrt{m}\eta$  and  $|u_i^T e| \approx \eta$ ,  $i = 1, 2, \dots, n$ ; see, e.g., [53, p.70-1] and [56, p.41-2]. The noise  $e$  thus affects  $u_i^T b$ ,  $i = 1, 2, \dots, n$ , *more or less equally*. With (1.6), relation (1.5) shows that for large singular values  $|u_i^T \hat{b}|/\sigma_i$  is dominant relative to  $|u_i^T e|/\sigma_i$ . Once  $|u_i^T \hat{b}| \leq |u_i^T e|$  from some  $i$  onwards, the small singular values magnify  $|u_i^T e|/\sigma_i$ , and the noise  $e$  dominates  $|u_i^T b|/\sigma_i$  and must be suppressed. The transition point  $k_0$  is such that

$$(1.7) \quad |u_{k_0}^T b| \approx |u_{k_0}^T \hat{b}| > |u_{k_0}^T e| \approx \eta, \quad |u_{k_0+1}^T b| \approx |u_{k_0+1}^T e| \approx \eta;$$

see [56, p.42, 98] and a similar description [53, p.70-1]. The  $\sigma_k$  are then divided into the  $k_0$  large ones and the  $n - k_0$  small ones. The truncated SVD (TSVD) method [53, 56] computes the TSVD regularized solutions

$$(1.8) \quad x_k^{tsvd} = \begin{cases} \sum_{i=1}^k \frac{u_i^T b}{\sigma_i} v_i \approx \sum_{i=1}^k \frac{u_i^T \hat{b}}{\sigma_i} v_i, & k \leq k_0; \\ \sum_{i=1}^k \frac{u_i^T b}{\sigma_i} v_i \approx \sum_{i=1}^{k_0} \frac{u_i^T \hat{b}}{\sigma_i} v_i + \sum_{i=k_0+1}^k \frac{u_i^T e}{\sigma_i} v_i, & k > k_0. \end{cases}$$

It is known from [53, p.70-1] and [56, p.86-8,96] that  $x_{k_0}^{tsvd}$  is the best TSVD regularized solution to (1.1) and balances the regularization and perturbation errors optimally. The parameter  $k$  is a regularization parameter that determines how many large SVD components of  $A$  are used to compute a regularized solution  $x_k^{tsvd}$  to (1.1).

Let  $U_k = (u_1, \dots, u_k)$ ,  $V_k = (v_1, \dots, v_k)$  and  $\Sigma_k = \text{diag}(\sigma_1, \dots, \sigma_k)$ , and define  $A_k = U_k \Sigma_k V_k^T$ . Then  $A_k$  is the best rank  $k$  approximation to  $A$  with  $\|A - A_k\| = \sigma_{k+1}$  (cf. [10, p.12]), and  $x_k^{tsvd} = A_k^\dagger b$  is the minimum-norm least squares solution to

$$\min_{x \in \mathbb{R}^n} \|A_k x - b\|$$

that perturbs  $A$  to  $A_k$  in (1.1). This interpretation will be often exploited later.

The solution  $x_\lambda$  of the Tikhonov regularization has a filtered SVD expansion

$$(1.9) \quad x_\lambda = \sum_{i=1}^n f_i \frac{u_i^T b}{\sigma_i} v_i,$$

where the  $f_i = \frac{\sigma_i^2}{\sigma_i^2 + \lambda^2}$  are called filters. The TSVD method is a special parameter filtered method, where, in  $x_k^{tsvd}$ , we take  $f_i = 1$ ,  $i = 1, 2, \dots, k$  and  $f_i = 0$ ,  $i = k + 1, \dots, n$ . The error  $x_\lambda - x_{true}$  can be written as the sum of the regularization and perturbation errors, and an optimal  $\lambda_{opt}$  aims to balance these two errors and make the sum of their norms minimized [53, 56, 81, 119]. The best possible regularized solution  $x_{\lambda_{opt}}$  retains the  $k_0$  dominant SVD components and dampens the other  $n - k_0$  small SVD components as much as possible [53, 56]. Apparently, the ability to acquire only the largest SVD components of  $A$  is fundamental in solving (1.1).

A number of parameter-choice methods have been developed for finding  $\lambda_{opt}$  or  $k_0$ , such as the discrepancy principle [88], the L-curve criterion, whose use goes back to Miller [87] and Lawson and Hanson [84] and is termed much later and studied in detail in [52, 58], and the generalized cross validation (GCV) [39, 120]; see, e.g., [5, 53, 56, 76, 78, 80, 92, 102, 119] for numerous comparisons. All parameter-choice methods aim to make  $f_i/\sigma_i$  not small for  $i = 1, 2, \dots, k_0$  and  $f_i/\sigma_i \approx 0$  for  $i = k_0 + 1, \dots, n$ . Each of these methods has its own merits and disadvantages, and

no one is absolutely reliable for all ill-posed problems. For example, some of the mentioned parameter-choice methods may fail to find accurate approximations to  $\lambda_{opt}$ ; see [46, 118] for an analysis on the L-curve method and [53] for some other parameter-choice methods. A further investigation on parameter-choice methods is not our concern in this paper.

The TSVD method is important in its own right. It and the standard-form Tikhonov regularization produce very similar solutions with essentially the minimum 2-norm error, i.e., the worst-case error [81, p.13]; see [117], [51], [53, p.109-11] and [56, Sections 4.2 and 4.4]. Indeed, for a linear compact equation  $Kx = g$  including (1.2) with the noisy  $g$  and true solution  $x_{true}(t)$ , under the source condition that its solution  $x_{true}(t) \in \mathcal{R}(K^*)$  or  $x_{true}(t) \in \mathcal{R}(K^*K)$ , the range of the adjoint  $K^*$  of  $K$  or that of  $K^*K$ , which amounts to assuming that  $x_{true}(t)$  or its derivative is squares integrable, the errors of the best regularized solutions by the TSVD method and the Tikhonov regularization are *order optimal, i.e., the same order as the worst-case error* [81, p.13,18,20,32-40], [90, p.90] and [119, p.7-12]. These conclusions carries over to (1.1) [119, p.8]. Therefore, either of  $x_{\lambda_{opt}}$  and  $x_{k_0}^{tsvd}$  is a best possible solution to (1.1) under the above assumptions and can be taken as standard reference when assessing the regularizing effects of an iterative solver. For the sake of clarity, we will take  $x_{k_0}^{tsvd}$ .

For (1.1) large, the TSVD method and the Tikhonov regularization method are generally too demanding, and only iterative regularization methods are computationally viable. A major class of methods has been Krylov iterative solvers that project (1.1) onto a sequence of low dimensional Krylov subspaces and computes iterates to approximate  $x_{true}$ ; see, e.g., [1, 27, 38, 45, 53, 56, 81]. Of Krylov iterative solvers, the CGLS (or CGNR) method, which implicitly applies the Conjugate Gradient (CG) method [40, 60] to the normal equations  $A^T A x = A^T b$  of (1.1), and its mathematically equivalent LSQR algorithm [98] have been most commonly used. The Krylov solvers CGME (or CGNE) [10, 11, 22, 45, 47, 61] and LSMR [11, 30] are also choices, which amount to the CG method applied to  $\min \|AA^T y - b\|$  with  $x = A^T y$  and MINRES [97] applied to  $A^T A x = A^T b$ , respectively. These Krylov solvers have been intensively studied and known to have regularizing effects [1, 24, 38, 45, 47, 53, 56, 61] and exhibit semi-convergence [90, p.89]; see also [10, p.314], [11, p.733], [53, p.135] and [56, p.110]: The iterates converge to  $x_{true}$  and their norms increase steadily, and the residual norms decrease in an initial stage; then afterwards the noise  $e$  starts to deteriorate the iterates so that they start to diverge from  $x_{true}$  and instead converge to  $x_{naive}$ , while their norms increase considerably and the residual norms stabilize. If we stop at the right time, then, in principle, we have a regularization method, where the iteration number plays the role of parameter regularization. Semi-convergence is due to the fact that the projected problem starts to inherit the ill-conditioning of (1.1) from some iteration onwards, and the appearance of a small singular value of the projected problem amplifies the noise considerably.

The regularizing effects of CG type methods were noticed by Lanczos [83] and were rediscovered in [74, 106, 110]. Based on these works and motivated by a heuristic explanation on good numerical results with very few iterations using CGLS in [74], and realizing that such an excellent performance can only be expected if convergence to the regular part of the solution, i.e.,  $x_{k_0}^{tsvd}$ , takes place before the effects of ill-posedness show up, on page 13 of [12], Björck and Eldén in 1979 foresightedly expressed a fundamental concern on CGLS (and LSQR): *More research is needed to tell for which problems this approach will work, and what stopping criterion to choose.* See also [53, p.145]. As remarked by Hanke and Hansen [48], the paper [12] was the only

extensive survey on algorithmic details until that time, and a strict proof of the regularizing properties of conjugate gradients is extremely difficult. An enormous effort has long been made to the study of regularizing effects of LSQR and CGLS (cf. [24, 27, 28, 37, 45, 47, 53, 56, 61, 81, 91, 94, 99, 105, 114]) in the Hilbert or finite dimensional space setting, but a rigorous regularization theory of LSQR and CGLS for (1.1) is still lacking, and there has been no definitive answer to the above long-standing fundamental question, and the same is for LSMR and CGME.

For  $A$  symmetric, MINRES and MR-II applied to  $Ax = b$  directly are alternatives and have been shown to have regularizing effects [17, 45, 49, 56, 67, 79], but MR-II seems preferable since the noisy  $b$  is excluded in the underlying subspace [65, 67]. For  $A$  nonsymmetric or multiplication with  $A^T$  difficult to compute, GMRES and RRGMR are candidate methods [3, 18, 19, 93], and the latter may be better [67]. The hybrid approaches based on the Arnoldi process have been first proposed in [20] and studied in [17, 21, 85, 95]. Gazzola and her coauthors [31]–[35] have described a general framework of the hybrid methods and presented various Krylov-Tikhonov methods with different parameter-choice strategies. Unfortunately, unlike LSQR and CGLS, these methods are highly problem dependent and may not have regularizing effects for general nonsymmetric ill-posed problems; see, e.g., [67] and [56, p.126]. The fundamental cause is that the underlying Krylov subspaces may not favor the dominant left and singular subspaces of  $A$ , which are desired in solving (1.1).

The behavior of ill-posed problems critically depends on the decay rate of  $\sigma_j$ . The following characterization of the degree of ill-posedness of (1.1) was introduced in [62] and has been widely used [1, 27, 53, 56, 89]: If  $\sigma_j = \mathcal{O}(j^{-\alpha})$ , then (1.1) is mildly or moderately ill-posed for  $\frac{1}{2} < \alpha \leq 1$  or  $\alpha > 1$ . If  $\sigma_j = \mathcal{O}(\rho^{-j})$  with  $\rho > 1$ ,  $j = 1, 2, \dots, n$ , then (1.1) is severely ill-posed. Here for mildly ill-posed problems we add the requirement  $\alpha > \frac{1}{2}$ , which does not appear in [62] but must be met for  $k(s, t) \in L^2(\Omega \times \Omega)$  in (1.1) [48, 53]. In the one-dimensional case, i.e.,  $q = 1$ , (1.1) is severely ill-posed with  $k(s, t)$  sufficiently smooth, and it is moderately ill-posed with  $\sigma_j = \mathcal{O}(j^{-p-1/2})$ , where  $p$  is the highest order of continuous derivatives of  $k(s, t)$ ; see, e.g., [53, p.8] and [56, p.10-11]. Clearly, the singular values  $\sigma_j$  for a severely ill-posed problem decay at the same rate  $\rho^{-1}$ , while those of a moderately or mildly ill-posed problem decay at the decreasing rate  $\left(\frac{j}{j+1}\right)^\alpha$  that approaches one more quickly with  $j$  for the mildly ill-posed problem than for the moderately ill-posed problem.

If a regularized solution to (1.1) is at least as accurate as  $x_{k_0}^{tsvd}$ , then it is called a best possible regularized solution. Given (1.1), if the regularized solution of an iterative regularization solver at semi-convergence is a best possible one, then, by the words of Björck and Eldén, the solver *works* for the problem and is said to have the *full* regularization. Otherwise, the solver is said to have the *partial* regularization.

Because it has been unknown whether or not LSQR, CGLS, LSMR and CGME have the full regularization for a given (1.1), one commonly combines them with some explicit regularization, so that the resulting hybrid variants (hopefully) find best possible regularized solutions [1, 53, 56]. A hybrid CGLS is to run CGLS for several trial regularization parameters  $\lambda$  and picks up the best one among the candidates [1]. Its disadvantages are that regularized solutions cannot be updated with different  $\lambda$  and there is no guarantee that the selected regularized solution is a best possible one. The hybrid LSQR variants have been advocated by Björck and Eldén [12] and O’Leary and Simmons [96], and improved and developed by Björck [9] and Björck, Grimme and Van Dooren [13]. A hybrid LSQR first projects (1.1) onto Krylov subspaces and then regularizes the projected problems explicitly. It aims to remove the effects of small

Ritz values and expands a Krylov subspace until it captures the  $k_0$  dominant SVD components of  $A$  [9, 13, 48, 96]. The hybrid LSQR and CGME have been intensively studied in, e.g., [6, 7, 8, 23, 47, 48, 85, 93, 95, 103] and [1, 56, 59]. Within the framework of such hybrid solvers, it is hard to find a near-optimal regularization parameter [13, 103]. More seriously, as we will elaborate mathematically and numerically in the concluding section of this paper, it may make no sense to speak of the regularization of the projected problems and their optimal regularization parameters since they may actually fail to satisfy the discrete Picard conditions. In contrast, if an iterative solver has the full regularization, we stop it after semi-convergence. Obviously, we cannot emphasize too much the importance of completely understanding the regularization of LSQR, CGLS, LSMR and CGME. By the definition of the full or partial regularization, we now modify the concern of Björck and Eldén as: *Do LSQR, CGLS, LSMR and CGME have the full or partial regularization for severely, moderately and mildly ill-posed problems? How to identify their full or partial regularization in practice?*

In this paper, assuming exact arithmetic, we first focus on LSQR and make a rigorous analysis on its regularization for severely, moderately and mildly ill-posed problems. Due to the mathematical equivalence of CGLS and LSQR, the assertions on the full or partial regularization of LSQR apply to CGLS as well. We then analyze the regularizing effects of LSMR and CGME and draw definitive conclusions. We prove that LSQR has the full regularization for severely and moderately ill-posed problems once  $\rho > 1$  and  $\alpha > 1$  suitably, and it generally has only the partial regularization for mildly ill-posed problems. In Section 2, we describe the Lanczos bidiagonalization process and LSQR, and make an introductory analysis. In Section 3, we establish accurate  $\sin \Theta$  theorems for the 2-norm distance between the underlying  $k$ -dimensional Krylov subspace and the  $k$ -dimensional dominant right singular subspace of  $A$ . We then derive some follow-up results that play a central role in analyzing the regularization of LSQR. In Section 4, we prove that a  $k$ -step Lanczos bidiagonalization always generates a near best rank  $k$  approximation to  $A$ , and the  $k$  Ritz values always approximate the first  $k$  large singular values in natural order, and no small Ritz value appears for  $k = 1, 2, \dots, k_0$ . This will show that LSQR has the full regularization. For mildly ill-posed problems, we prove that, for some  $k \leq k_0$ , the  $k$  Ritz values generally do not approximate the first  $k$  large singular values in natural order and LSQR generally has only the partial regularization. In Section 5, we derive bounds for the entries of bidiagonal matrices generated by Lanczos bidiagonalization, proving how fast they decay and showing how to use them to reliably identify if LSQR has the full regularization when the degree of ill-posedness of (1.1) is unknown in advance. Exploiting some of the results on LSQR, we analyze the regularization of LSMR and CGME and prove that LSMR has similar regularizing effects to LSQR for each kind of problem and both of them are superior to CGME. In Section 6, we present some perturbation results and prove that LSQR resembles the TSVD method for severely and moderately ill-posed problems. In Section 7, with a number of nontrivial changes and reformulations, we extend all the results to the case that  $A$  has multiple singular values. In Section 8, we report numerical experiments to confirm our theory on LSQR. Finally, we summarize the paper with further remarks in Section 9.

Throughout the paper, denote by  $\mathcal{K}_k(C, w) = \text{span}\{w, Cw, \dots, C^{k-1}w\}$  the  $k$ -dimensional Krylov subspace generated by the matrix  $C$  and the vector  $w$ , and by  $I$  and the bold letter  $\mathbf{0}$  the identity matrix and the zero matrix with orders clear from the context, respectively. For  $B = (b_{ij})$ , we define the nonnegative matrix  $|B| = (|b_{ij}|)$ , and for  $|C| = (|c_{ij}|)$ ,  $|B| \leq |C|$  means  $|b_{ij}| \leq |c_{ij}|$  componentwise.



**2. The LSQR algorithm.** LSQR is based on the Lanczos bidiagonalization process, which computes two orthonormal bases  $\{q_1, q_2, \dots, q_k\}$  and  $\{p_1, p_2, \dots, p_{k+1}\}$  of  $\mathcal{K}_k(A^T A, A^T b)$  and  $\mathcal{K}_{k+1}(AA^T, b)$  for  $k = 1, 2, \dots, n$ , respectively. We describe the process as Algorithm 1.

**Algorithm 1:  $k$ -step Lanczos bidiagonalization process**

1. Take  $p_1 = b/\|b\| \in \mathbb{R}^m$ , and define  $\beta_1 q_0 = 0$ .
2. For  $j = 1, 2, \dots, k$ 
  - (i)  $r = A^T p_j - \beta_j q_{j-1}$
  - (ii)  $\alpha_j = \|r\|$ ;  $q_j = r/\alpha_j$
  - (iii)  $z = Aq_j - \alpha_j p_j$
  - (iv)  $\beta_{j+1} = \|z\|$ ;  $p_{j+1} = z/\beta_{j+1}$ .

Algorithm 1 can be written in the matrix form

$$(2.1) \quad AQ_k = P_{k+1} B_k,$$

$$(2.2) \quad A^T P_{k+1} = Q_k B_k^T + \alpha_{k+1} q_{k+1} e_{k+1}^T.$$

where  $e_{k+1}$  denotes the  $(k+1)$ -th canonical basis vector of  $\mathbb{R}^{k+1}$ ,  $P_{k+1} = (p_1, p_2, \dots, p_{k+1})$ ,  $Q_k = (q_1, q_2, \dots, q_k)$  and

$$(2.3) \quad B_k = \begin{pmatrix} \alpha_1 & & & \\ \beta_2 & \alpha_2 & & \\ & \beta_3 & \ddots & \\ & & \ddots & \alpha_k \\ & & & \beta_{k+1} \end{pmatrix} \in \mathbb{R}^{(k+1) \times k}.$$

It is known from (2.1) that

$$(2.4) \quad B_k = P_{k+1}^T A Q_k.$$

We remind that the singular values of  $B_k$ , called the Ritz values of  $A$  with respect to the left and right subspaces  $\text{span}\{P_{k+1}\}$  and  $\text{span}\{Q_k\}$ , are all simple. This basic fact will often be used later.

At iteration  $k$ , LSQR solves the problem  $\|Ax^{(k)} - b\| = \min_{x \in \mathcal{K}_k(A^T A, A^T b)} \|Ax - b\|$  and computes the iterates  $x^{(k)} = Q_k y^{(k)}$  with

$$(2.5) \quad y^{(k)} = \arg \min_{y \in \mathbb{R}^k} \|B_k y - \|b\| e_1^{(k+1)}\| = \|b\| B_k^\dagger e_1^{(k+1)},$$

where  $e_1^{(k+1)}$  is the first canonical basis vector of  $\mathbb{R}^{k+1}$ , and the residual norm  $\|Ax^{(k)} - b\|$  decreases monotonically with respect to  $k$ . We have  $\|Ax^{(k)} - b\| = \|B_k y^{(k)} - \|b\| e_1^{(k+1)}\|$  and  $\|x^{(k)}\| = \|y^{(k)}\|$ , both of which can be cheaply computed.

Note that  $\|b\| e_1^{(k+1)} = P_{k+1}^T b$ . We have

$$(2.6) \quad x^{(k)} = Q_k B_k^\dagger P_{k+1}^T b,$$

that is, the iterate  $x^{(k)}$  by LSQR is the minimum-norm least squares solution to the perturbed problem that replaces  $A$  in (1.1) by its rank  $k$  approximation  $P_{k+1} B_k Q_k^T$ . Recall that the best rank  $k$  approximation  $A_k$  to  $A$  satisfies  $\|A - A_k\| = \sigma_{k+1}$ . We can relate LSQR and the TSVD method from two perspectives. One of them is to interpret LSQR as solving a nearby problem that perturbs  $A_k$  to  $P_{k+1} B_k Q_k^T$ , provided that

$P_{k+1}B_kQ_k^T$  is a near best rank  $k$  approximation to  $A$  with an approximate accuracy  $\sigma_{k+1}$ . The other is to interpret  $x_k^{tsvd}$  and  $x^{(k)}$  as the solutions to the two perturbed problems of (1.1) that replace  $A$  by the rank  $k$  approximations with the same quality to  $A$ , respectively. Both perspectives lead to the consequence: the LSQR iterate  $x^{(k_0)}$  is as accurate as  $x_{k_0}^{tsvd}$  and is thus a best possible regularized solution to (1.1), provided that  $P_{k+1}B_kQ_k^T$  is a near best rank  $k$  approximation to  $A$  with the approximate accuracy  $\sigma_{k+1}$  and the  $k$  singular values of  $B_k$  approximate the first  $k$  large ones of  $A$  in natural order for  $k = 1, 2, \dots, k_0$ . Otherwise, as will be clear later,  $x^{(k_0)}$  cannot be as accurate as  $x_{k_0}^{tsvd}$  if either  $P_{k_0+1}B_{k_0}Q_{k_0}^T$  is not a near best rank  $k_0$  approximation to  $A$  or  $B_{k_0}$  has at least one singular value smaller than  $\sigma_{k_0+1}$ . We will give a precise definition of a near best rank  $k$  approximation later.

As stated in the introduction, the semi-convergence of LSQR must occur at some iteration  $k$ . Under the discrete Picard condition (1.6), if semi-convergence occurs at iteration  $k_0$ , we are sure that LSQR has the full regularization because  $x^{(k_0)}$  has captured the  $k_0$  dominant SVD components of  $A$  and effectively suppressed the other  $n - k_0$  SVD components; if semi-convergence occurs at some iteration  $k < k_0$ , then LSQR has only the partial regularization since it has not yet captured the needed  $k_0$  dominant SVD components of  $A$ .

**3.  $\sin \Theta$  theorems for the distances between  $\mathcal{K}_k(A^T A, A^T b)$  and  $\text{span}\{V_k\}$  as well as the others related.** Van der Sluis and Van der Vorst [113] prove the following result, which has been used in Hansen [53] and the references therein to illustrate and analyze the regularizing effects of LSQR and CGLS. We will also investigate it further in our paper.

**PROPOSITION 3.1.** *LSQR with the starting vector  $p_1 = b/\|b\|$  and CGLS applied to  $A^T A x = A^T b$  with the starting vector  $x^{(0)} = 0$  generate the same iterates*

$$(3.1) \quad x^{(k)} = \sum_{i=1}^n f_i^{(k)} \frac{u_i^T b}{\sigma_i} v_i, \quad k = 1, 2, \dots, n,$$

where

$$(3.2) \quad f_i^{(k)} = 1 - \prod_{j=1}^k \frac{(\theta_j^{(k)})^2 - \sigma_i^2}{(\theta_j^{(k)})^2}, \quad i = 1, 2, \dots, n,$$

and the  $\theta_j^{(k)}$  are the singular values of  $B_k$  labeled as  $\theta_1^{(k)} > \theta_2^{(k)} > \dots > \theta_k^{(k)}$ .

(3.1) shows that  $x^{(k)}$  has a filtered SVD expansion of form (1.9). If all the Ritz values  $\theta_j^{(k)}$  approximate the first  $k$  singular values  $\sigma_j$  of  $A$  in natural order, the filters  $f_i^{(k)} \approx 1$ ,  $i = 1, 2, \dots, k$  and the other  $f_i^{(k)}$  monotonically decay to zero for  $i = k+1, k+2, \dots, n$ . If this is the case until  $k = k_0$ , the  $k_0$ -step LSQR has the full regularization and computes a best possible regularized solution  $x^{(k_0)}$ . However, if a small Ritz value appears before some  $k \leq k_0$ , i.e.,  $\theta_{k-1}^{(k)} > \sigma_{k_0+1}$  and  $\sigma_{j^*} < \theta_k^{(k)} \leq \sigma_{k_0+1}$  with the smallest integer  $j^* > k_0 + 1$ , then  $f_i^{(k)} \in (0, 1)$  tends to zero monotonically for  $i = j^*, j^* + 1, \dots, n$ ; on the other hand, we have

$$\prod_{j=1}^k \frac{(\theta_j^{(k)})^2 - \sigma_i^2}{(\theta_j^{(k)})^2} = \frac{(\theta_k^{(k)})^2 - \sigma_i^2}{(\theta_k^{(k)})^2} \prod_{j=1}^{k-1} \frac{(\theta_j^{(k)})^2 - \sigma_i^2}{(\theta_j^{(k)})^2} \leq 0, \quad i = k_0 + 1, \dots, j^* - 1$$

since the first factor is non-positive and the second factor is positive. Then we get  $f_i^{(k)} \geq 1$ ,  $i = k_0 + 1, \dots, j^* - 1$ , so that  $x^{(k)}$  is deteriorated and LSQR has only



the partial regularization. Hansen [53, p.146-157] summarizes the known results on  $f_i^{(k)}$ , where a bound for  $|f_i^{(k)} - 1|$ ,  $i = 1, 2, \dots, k$  is given in [53, p.155] but there is no accurate estimate for the bound. As we will see in Section 6, the results to be established in this paper can be used for this purpose, and, more importantly, we will show that the bound in [53, p.155] can be sharpened substantially.

The standard  $k$ -step Lanczos bidiagonalization method computes the  $k$  Ritz values  $\theta_j^{(k)}$ , which are used to approximate some of the singular values of  $A$ , and is mathematically equivalent to the symmetric Lanczos method for the eigenvalue problem of  $A^T A$  starting with  $q_1 = A^T b / \|A^T b\|$ ; see [10, 11] or [2, 71, 72] for several variations that are based on standard, harmonic, refined projection [4, 108, 115] or a combination of them. A general convergence theory of harmonic and refined harmonic projection methods was lacking in the books [4, 108, 115] and has later been established in [70]. As is known from [10, 86, 100], for a general singular value distribution and a general vector  $b$ , some of the  $k$  Ritz values become good approximations to the largest and smallest singular values of  $A$  as  $k$  increases. If large singular values are well separated but small singular values are clustered, large Ritz values converge fast but small Ritz values converge very slowly.

For (1.1), we see from (1.4) and (1.6) that  $A^T b$  contains more information on dominant right singular vectors than on the ones corresponding to small singular values. Therefore,  $\mathcal{K}_k(A^T A, A^T b)$  hopefully contains richer information on the first  $k$  right singular vectors  $v_i$  than on the other  $n-k$  ones, at least for  $k$  small. Furthermore, note that  $A$  has many small singular values clustered at zero. Due to these two basic facts, all the Ritz values are expected to approximate the large singular values of  $A$  in natural order until some iteration  $k$ , at which a small Ritz value shows up and the regularized solutions then start to be contaminated by the noise  $e$  dramatically after that iteration. These qualitative arguments are frequently used to analyze and elaborate the regularizing effects of LSQR and CGLS; see, e.g., [1, 53, 55, 56, 59] and the references therein. Clearly, these arguments are not precise and cannot help us draw any definitive conclusion on the full or partial regularization of LSQR. For a severely ill-posed example from seismic tomography, it is reported in [114] that the desired convergence of the Ritz values actually holds as long as the discrete Picard condition is satisfied and there is a good separation among the large singular values of  $A$ . Unfortunately, there has been no mathematical justification on these observations.

A complete understanding of the regularization of LSQR includes accurate solutions of the following basic problems: How well or accurately does  $\mathcal{K}_k(A^T A, A^T b)$  approximate or capture the  $k$ -dimensional dominant right singular subspace of  $A$ ? How accurate is the rank  $k$  approximation  $P_{k+1} B_k Q_k^T$  to  $A$ ? Can it be a near best rank  $k$  approximation to  $A$ ? How does the noise level  $\|e\|$  affects the approximation accuracy of  $\mathcal{K}_k(A^T A, A^T b)$  and  $P_{k+1} B_k Q_k^T$  for  $k \leq k_0$  and  $k > k_0$ , respectively? What sufficient conditions on  $\rho$  and  $\alpha$  are needed to guarantee that  $P_{k+1} B_k Q_k^T$  is a near best rank  $k$  approximation to  $A$ ? When do the Ritz values  $\theta_i^{(k)}$  approximate  $\sigma_i$ ,  $i = 1, 2, \dots, k$  in natural order? When does at least a small Ritz value appear, i.e.,  $\theta_k^{(k)} < \sigma_{k_0+1}$  before some  $k \leq k_0$ ? We will make a rigorous and detailed analysis on these problems and some others related closely, present our results, and draw definitive assertions on the regularization of LSQR for three kinds of ill-posed problems.

In terms of the canonical angles  $\Theta(\mathcal{X}, \mathcal{Y})$  between two subspaces  $\mathcal{X}$  and  $\mathcal{Y}$  of the same dimension [109, p.43], we first present the following  $\sin \Theta$  theorem, showing how the  $k$ -dimensional Krylov subspace  $\mathcal{K}_k(A^T A, A^T b)$  captures or approximates the

$k$ -dimensional dominant right singular subspace of  $A$  for severely ill-posed problems.

**THEOREM 3.1.** *Let the SVD of  $A$  be as (1.4). Assume that (1.1) is severely ill-posed with  $\sigma_j = \mathcal{O}(\rho^{-j})$  and  $\rho > 1$ ,  $j = 1, 2, \dots, n$ , and the discrete Picard condition (1.6) is satisfied. Let  $\mathcal{V}_k = \text{span}\{V_k\}$  be the  $k$ -dimensional dominant right singular subspace of  $A$  spanned by the columns of  $V_k = (v_1, v_2, \dots, v_k)$  and  $\mathcal{V}_k^R = \mathcal{K}_k(A^T A, A^T b)$ . Then for  $k = 1, 2, \dots, n-1$  we have*

$$(3.3) \quad \|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\| = \frac{\|\Delta_k\|}{\sqrt{1 + \|\Delta_k\|^2}}$$

with  $\Delta_k \in \mathbb{R}^{(n-k) \times k}$  to be defined by (3.11) and

$$(3.4) \quad \|\Delta_1\| \leq \frac{\sigma_2}{\sigma_1} \frac{|u_2^T b|}{|u_1^T b|} (1 + \mathcal{O}(\rho^{-2})),$$

$$(3.5) \quad \|\Delta_k\| \leq \frac{\sigma_{k+1}}{\sigma_k} \frac{|u_{k+1}^T b|}{|u_k^T b|} (1 + \mathcal{O}(\rho^{-2})) |L_{k_1}^{(k)}(0)|, \quad k = 2, 3, \dots, n-1,$$

where

$$(3.6) \quad |L_{k_1}^{(k)}(0)| = \max_{j=1,2,\dots,k} |L_j^{(k)}(0)|, \quad |L_j^{(k)}(0)| = \prod_{i=1, i \neq j}^k \frac{\sigma_i^2}{|\sigma_j^2 - \sigma_i^2|}, \quad j = 1, 2, \dots, k.$$

In particular, we have

$$(3.7) \quad \|\Delta_1\| \leq \frac{\sigma_2^{2+\beta}}{\sigma_1^{2+\beta}} (1 + \mathcal{O}(\rho^{-2})),$$

$$(3.8) \quad \|\Delta_k\| \leq \frac{\sigma_{k+1}^{2+\beta}}{\sigma_k^{2+\beta}} (1 + \mathcal{O}(\rho^{-2})) |L_{k_1}^{(k)}(0)|, \quad k = 2, 3, \dots, k_0,$$

$$(3.9) \quad \|\Delta_k\| \leq \frac{\sigma_{k+1}}{\sigma_k} (1 + \mathcal{O}(\rho^{-2})) |L_{k_1}^{(k)}(0)|, \quad k = k_0 + 1, \dots, n-1.$$

*Proof.* Let  $U_n = (u_1, u_2, \dots, u_n)$  whose columns are the first  $n$  left singular vectors of  $A$  defined by (1.4). Then the Krylov subspace  $\mathcal{K}_k(\Sigma^2, \Sigma U_n^T b) = \text{span}\{DT_k\}$  with

$$D = \text{diag}(\sigma_i u_i^T b) \in \mathbb{R}^{n \times n}, \quad T_k = \begin{pmatrix} 1 & \sigma_1^2 & \dots & \sigma_1^{2k-2} \\ 1 & \sigma_2^2 & \dots & \sigma_2^{2k-2} \\ \vdots & \vdots & & \vdots \\ 1 & \sigma_n^2 & \dots & \sigma_n^{2k-2} \end{pmatrix}.$$

Partition the diagonal matrix  $D$  and the matrix  $T_k$  as follows:

$$D = \begin{pmatrix} D_1 & 0 \\ 0 & D_2 \end{pmatrix}, \quad T_k = \begin{pmatrix} T_{k1} \\ T_{k2} \end{pmatrix},$$

where  $D_1, T_{k1} \in \mathbb{R}^{k \times k}$ . Since  $T_{k1}$  is a Vandermonde matrix with  $\sigma_j$  supposed to be distinct for  $j = 1, 2, \dots, k$ , it is nonsingular. Therefore, from  $\mathcal{K}_k(A^T A, A^T b) = \text{span}\{VDT_k\}$  we have

$$(3.10) \quad \mathcal{V}_k^R = \mathcal{K}_k(A^T A, A^T b) = \text{span} \left\{ V \begin{pmatrix} D_1 T_{k1} \\ D_2 T_{k2} \end{pmatrix} \right\} = \text{span} \left\{ V \begin{pmatrix} I \\ \Delta_k \end{pmatrix} \right\},$$

where

$$(3.11) \quad \Delta_k = D_2 T_{k2} T_{k1}^{-1} D_1^{-1} \in \mathbb{R}^{(n-k) \times k}.$$

Write  $V = (V_k, V_k^\perp)$ , and define

$$(3.12) \quad Z_k = V \begin{pmatrix} I \\ \Delta_k \end{pmatrix} = V_k + V_k^\perp \Delta_k.$$

Then  $Z_k^T Z_k = I + \Delta_k^T \Delta_k$ , and the columns of  $\hat{Z}_k = Z_k (Z_k^T Z_k)^{-\frac{1}{2}}$  form an orthonormal basis of  $\mathcal{V}_k^R$ . So we get an orthogonal direct sum decomposition of  $\hat{Z}_k$ :

$$(3.13) \quad \hat{Z}_k = (V_k + V_k^\perp \Delta_k)(I + \Delta_k^T \Delta_k)^{-\frac{1}{2}}.$$

By definition and (3.13), for the matrix 2-norm we obtain

$$(3.14) \quad \|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\| = \|(V_k^\perp)^T \hat{Z}_k\| = \|\Delta_k (I + \Delta_k^T \Delta_k)^{-\frac{1}{2}}\| = \frac{\|\Delta_k\|}{\sqrt{1 + \|\Delta_k\|^2}},$$

which is (3.3).

Next we estimate  $\|\Delta_k\|$ . For  $k = 2, 3, \dots, n-1$ , it is easily justified that the  $j$ -th column of  $T_{k1}^{-1}$  consists of the coefficients of the  $j$ -th Lagrange polynomial

$$L_j^{(k)}(\lambda) = \prod_{i=1, i \neq j}^k \frac{\lambda - \sigma_i^2}{\sigma_j^2 - \sigma_i^2}$$

that interpolates the elements of the  $j$ -th canonical basis vector  $e_j^{(k)} \in \mathbb{R}^k$  at the abscissas  $\sigma_1^2, \sigma_2^2, \dots, \sigma_k^2$ . Consequently, the  $j$ -th column of  $T_{k2} T_{k1}^{-1}$  is

$$(3.15) \quad T_{k2} T_{k1}^{-1} e_j^{(k)} = (L_j^{(k)}(\sigma_{k+1}^2), \dots, L_j^{(k)}(\sigma_n^2))^T, \quad j = 1, 2, \dots, k,$$

from which we obtain

$$(3.16) \quad T_{k2} T_{k1}^{-1} = \begin{pmatrix} L_1^{(k)}(\sigma_{k+1}^2) & L_2^{(k)}(\sigma_{k+1}^2) & \dots & L_k^{(k)}(\sigma_{k+1}^2) \\ L_1^{(k)}(\sigma_{k+2}^2) & L_2^{(k)}(\sigma_{k+2}^2) & \dots & L_k^{(k)}(\sigma_{k+2}^2) \\ \vdots & \vdots & \ddots & \vdots \\ L_1^{(k)}(\sigma_n^2) & L_2^{(k)}(\sigma_n^2) & \dots & L_k^{(k)}(\sigma_n^2) \end{pmatrix} \in \mathbb{R}^{(n-k) \times k}.$$

Since  $|L_j^{(k)}(\lambda)|$  is monotonically decreasing for  $0 \leq \lambda < \sigma_k^2$ , it is bounded by  $|L_j^{(k)}(0)|$ .

With this property and the definition of  $L_{k1}^{(k)}(0)$  by (3.6), we get

$$(3.17) \quad \begin{aligned} |\Delta_k| &= |D_2 T_{k2} T_{k1}^{-1} D_1^{-1}| \\ &\leq \begin{pmatrix} \frac{\sigma_{k+1}}{\sigma_1} \left| \frac{u_{k+1}^T b}{u_1^T b} \right| |L_{k1}^{(k)}(0)|, & \frac{\sigma_{k+1}}{\sigma_2} \left| \frac{u_{k+1}^T b}{u_2^T b} \right| |L_{k1}^{(k)}(0)|, & \dots & \frac{\sigma_{k+1}}{\sigma_k} \left| \frac{u_{k+1}^T b}{u_k^T b} \right| |L_{k1}^{(k)}(0)| \\ \frac{\sigma_{k+2}}{\sigma_1} \left| \frac{u_{k+2}^T b}{u_1^T b} \right| |L_{k1}^{(k)}(0)|, & \frac{\sigma_{k+2}}{\sigma_2} \left| \frac{u_{k+2}^T b}{u_2^T b} \right| |L_{k1}^{(k)}(0)|, & \dots & \frac{\sigma_{k+2}}{\sigma_k} \left| \frac{u_{k+2}^T b}{u_k^T b} \right| |L_{k1}^{(k)}(0)| \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\sigma_n}{\sigma_1} \left| \frac{u_n^T b}{u_1^T b} \right| |L_{k1}^{(k)}(0)|, & \frac{\sigma_n}{\sigma_2} \left| \frac{u_n^T b}{u_2^T b} \right| |L_{k1}^{(k)}(0)|, & \dots & \frac{\sigma_n}{\sigma_k} \left| \frac{u_n^T b}{u_k^T b} \right| |L_{k1}^{(k)}(0)| \end{pmatrix} \\ &= |L_{k1}^{(k)}(0)| |\tilde{\Delta}_k|, \end{aligned}$$

where

$$(3.18) \quad |\tilde{\Delta}_k| = \left| (\sigma_{k+1} u_{k+1}^T b, \sigma_{k+2} u_{k+2}^T b, \dots, \sigma_n u_n^T b)^T \left( \frac{1}{\sigma_1 u_1^T b}, \frac{1}{\sigma_2 u_2^T b}, \dots, \frac{1}{\sigma_k u_k^T b} \right) \right|$$

is a rank one matrix. Therefore, by  $\|C\| \leq \| |C| \|$  (cf. [107, p.53]), we get

$$(3.19) \quad \begin{aligned} \|\Delta_k\| &\leq \| |\Delta_k| \| \leq |L_{k_1}^{(k)}(0)| \left\| |\tilde{\Delta}_k| \right\| \\ &= |L_{k_1}^{(k)}(0)| \left( \sum_{j=k+1}^n \sigma_j^2 |u_j^T b|^2 \right)^{1/2} \left( \sum_{j=1}^k \frac{1}{\sigma_j^2 |u_j^T b|^2} \right)^{1/2}. \end{aligned}$$

By the discrete Picard condition (1.6), (1.7) and the description between them, for the white noise  $e$ , it is known from [53, p.70-1] and [56, p.41-2] that  $|u_j^T b| \approx |u_j^T \hat{b}| = \sigma_j^{1+\beta}$  decrease as  $j$  increases up to  $k_0$  and then become stabilized as  $|u_j^T b| \approx |u_j^T e| \approx \eta \approx \frac{\|e\|}{\sqrt{m}}$ , a small constant for  $j > k_0$ . In order to simplify the derivation and present our results compactly, in terms of these assumptions and properties, in later proofs we will use the following precise equalities and inequalities:

$$(3.20) \quad |u_j^T b| = |u_j^T \hat{b}| = \sigma_j^{1+\beta}, \quad j = 1, 2, \dots, k_0,$$

$$(3.21) \quad |u_j^T b| = |u_j^T e| = \eta, \quad j = k_0 + 1, \dots, n,$$

$$(3.22) \quad |u_{j+1}^T b| \leq |u_j^T b|, \quad j = 1, 2, \dots, n-1.$$

From (3.22) and  $\sigma_j = \mathcal{O}(\rho^{-j})$ ,  $j = 1, 2, \dots, n$ , for  $k = 1, 2, \dots, n-1$  we obtain

$$(3.23) \quad \begin{aligned} \left( \sum_{j=k+1}^n \sigma_j^2 |u_j^T b|^2 \right)^{1/2} &= \sigma_{k+1} |u_{k+1}^T b| \left( \sum_{j=k+1}^n \frac{\sigma_j^2 |u_j^T b|^2}{\sigma_{k+1}^2 |u_{k+1}^T b|^2} \right)^{1/2} \\ &\leq \sigma_{k+1} |u_{k+1}^T b| \left( \sum_{j=k+1}^n \frac{\sigma_j^2}{\sigma_{k+1}^2} \right)^{1/2} \\ &= \sigma_{k+1} |u_{k+1}^T b| \left( 1 + \sum_{j=k+2}^n \mathcal{O}(\rho^{2(k-j)+2}) \right)^{1/2} \\ &= \sigma_{k+1} |u_{k+1}^T b| \left( 1 + \mathcal{O} \left( \sum_{j=k+2}^n \rho^{2(k-j)+2} \right) \right)^{1/2} \\ &= \sigma_{k+1} |u_{k+1}^T b| \left( 1 + \mathcal{O} \left( \frac{\rho^{-2}}{1 - \rho^{-2}} (1 - \rho^{-2(n-k-1)}) \right) \right)^{1/2} \\ &= \sigma_{k+1} |u_{k+1}^T b| (1 + \mathcal{O}(\rho^{-2}))^{1/2} \\ &= \sigma_{k+1} |u_{k+1}^T b| (1 + \mathcal{O}(\rho^{-2})) \end{aligned}$$

with  $1 + \mathcal{O}(\rho^{-2})$  replaced by one for  $k = n-1$ . In a similar manner, for  $k =$

$2, 3, \dots, n-1$ , from (3.22) we get

$$\begin{aligned} \left( \sum_{j=1}^k \frac{1}{\sigma_j^2 |u_j^T b|^2} \right)^{1/2} &= \frac{1}{\sigma_k |u_k^T b|} \left( \sum_{j=1}^k \frac{\sigma_k^2 |u_k^T b|^2}{\sigma_j^2 |u_j^T b|^2} \right)^{1/2} \leq \frac{1}{\sigma_k |u_k^T b|} \left( \sum_{j=1}^k \frac{\sigma_k^2}{\sigma_j^2} \right)^{1/2} \\ &= \frac{1}{\sigma_k |u_k^T b|} \left( 1 + \mathcal{O} \left( \sum_{j=1}^{k-1} \rho^{2(j-k)} \right) \right)^{1/2} \\ &= \frac{1}{\sigma_k |u_k^T b|} (1 + \mathcal{O}(\rho^{-2})). \end{aligned}$$

From the above and (3.19), we finally obtain

$$\|\Delta_k\| \leq \frac{\sigma_{k+1}}{\sigma_k} \frac{|u_{k+1}^T b|}{|u_k^T b|} (1 + \mathcal{O}(\rho^{-2})) |L_{k_1}^{(k)}(0)|, \quad k = 2, 3, \dots, n-1,$$

which proves (3.5).

Note that the Langrange polynomials  $L_j^{(k)}(\lambda)$  require  $k \geq 2$ . So, we need to treat the case  $k = 1$  independently: from (3.11) and (3.22), observe that

$$T_{k2} = (1, 1, \dots, 1)^T, \quad D_2 T_{k2} = (\sigma_2 u_2^T b, \sigma_3 u_3^T b, \dots, \sigma_n u_n^T b)^T, \quad T_{k1}^{-1} = 1, \quad D_1^{-1} = \frac{1}{\sigma_1 u_1^T b}.$$

Therefore, we have

$$(3.24) \quad \Delta_1 = (\sigma_2 u_2^T b, \sigma_3 u_3^T b, \dots, \sigma_n u_n^T b)^T \frac{1}{\sigma_1 u_1^T b},$$

from which and (3.23) for  $k = 1$  it is direct to get (3.4).

In terms of the discrete Picard condition (1.6), (1.7), (3.20) and (3.21), we have

$$(3.25) \quad \frac{|u_{k+1}^T b|}{|u_k^T b|} = \frac{|u_{k+1}^T \hat{b}|}{|u_k^T \hat{b}|} = \frac{\sigma_{k+1}^{1+\beta}}{\sigma_k^{1+\beta}}, \quad k \leq k_0$$

and

$$(3.26) \quad \frac{|u_{k+1}^T b|}{|u_k^T b|} = \frac{|u_{k+1}^T e|}{|u_k^T e|} = 1, \quad k > k_0.$$

Applying them to (3.4) and (3.5) establishes (3.7), (3.8) and (3.9), respectively.  $\square$

We next estimate the factor  $|L_{k_1}^{(k)}(0)|$  accurately.

**THEOREM 3.2.** *For the severely ill-posed problem and  $k = 2, 3, \dots, n-1$ , we have*

$$(3.27) \quad |L_k^{(k)}(0)| = 1 + \mathcal{O}(\rho^{-2}),$$

$$(3.28) \quad |L_j^{(k)}(0)| = \frac{1 + \mathcal{O}(\rho^{-2})}{\prod_{i=j+1}^k \left( \frac{\sigma_i}{\sigma_j} \right)^2} = \frac{1 + \mathcal{O}(\rho^{-2})}{\mathcal{O}(\rho^{(k-j)(k-j+1)})}, \quad j = 1, 2, \dots, k-1,$$

$$(3.29) \quad |L_{k_1}^{(k)}(0)| = \max_{j=1,2,\dots,k} |L_j^{(k)}(0)| = 1 + \mathcal{O}(\rho^{-2}).$$

*Proof.* Exploiting the Taylor series expansion and  $\sigma_i = \mathcal{O}(\rho^{-i})$  for  $i = 1, 2, \dots, n$ , by definition, for  $j = 1, 2, \dots, k-1$  we have

$$\begin{aligned}
 |L_j^{(k)}(0)| &= \prod_{i=1, i \neq j}^k \left| \frac{\sigma_i^2}{\sigma_i^2 - \sigma_j^2} \right| = \prod_{i=1}^{j-1} \frac{\sigma_i^2}{\sigma_i^2 - \sigma_j^2} \cdot \prod_{i=j+1}^k \frac{\sigma_i^2}{\sigma_j^2 - \sigma_i^2} \\
 &= \prod_{i=1}^{j-1} \frac{1}{1 - \mathcal{O}(\rho^{-2(j-i)})} \prod_{i=j+1}^k \frac{1}{1 - \mathcal{O}(\rho^{-2(i-j)})} \frac{1}{\prod_{i=j+1}^k \mathcal{O}(\rho^{2(i-j)})} \\
 (3.30) \quad &= \frac{\left(1 + \sum_{i=1}^j \mathcal{O}(\rho^{-2i})\right) \left(1 + \sum_{i=1}^{k-j+1} \mathcal{O}(\rho^{-2i})\right)}{\prod_{i=j+1}^k \mathcal{O}(\rho^{2(i-j)})}
 \end{aligned}$$

by absorbing those higher order terms into the two  $\mathcal{O}(\cdot)$  in the numerator. For  $j = k$ , we get

$$\begin{aligned}
 |L_k^{(k)}(0)| &= \prod_{i=1}^{k-1} \left| \frac{\sigma_i^2}{\sigma_i^2 - \sigma_k^2} \right| = \prod_{i=1}^{k-1} \frac{1}{1 - \mathcal{O}(\rho^{-2(k-i)})} = \prod_{i=1}^{k-1} \frac{1}{1 - \mathcal{O}(\rho^{-2i})} \\
 &= 1 + \sum_{i=1}^k \mathcal{O}(\rho^{-2i}) = 1 + \mathcal{O}\left(\sum_{i=1}^k \rho^{-2i}\right) \\
 &= 1 + \mathcal{O}\left(\frac{\rho^{-2}}{1 - \rho^{-2}}(1 - \rho^{-2k})\right) = 1 + \mathcal{O}(\rho^{-2}),
 \end{aligned}$$

which is (3.27).

Note that for the numerator of (3.30) we have

$$1 + \sum_{i=1}^j \mathcal{O}(\rho^{-2i}) = 1 + \mathcal{O}\left(\sum_{i=1}^j \rho^{-2i}\right) = 1 + \mathcal{O}\left(\frac{\rho^{-2}}{1 - \rho^{-2}}(1 - \rho^{-2j})\right),$$

and

$$1 + \sum_{i=1}^{k-j+1} \mathcal{O}(\rho^{-2i}) = 1 + \mathcal{O}\left(\sum_{i=1}^{k-j+1} \rho^{-2i}\right) = 1 + \mathcal{O}\left(\frac{\rho^{-2}}{1 - \rho^{-2}}(1 - \rho^{-2(k-j+1)})\right),$$

whose product for any  $k$  is

$$1 + \mathcal{O}\left(\frac{2\rho^{-2}}{1 - \rho^{-2}}\right) + \mathcal{O}\left(\left(\frac{\rho^{-2}}{1 - \rho^{-2}}\right)^2\right) = 1 + \mathcal{O}\left(\frac{2\rho^{-2}}{1 - \rho^{-2}}\right) = 1 + \mathcal{O}(\rho^{-2}).$$

On the other hand, note that the denominator of (3.30) is defined by

$$\prod_{i=j+1}^k \left(\frac{\sigma_j}{\sigma_i}\right)^2 = \prod_{i=j+1}^k \mathcal{O}(\rho^{2(i-j)}) = \mathcal{O}((\rho \cdot \rho^2 \cdots \rho^{k-j})^2) = \mathcal{O}(\rho^{(k-j)(k-j+1)}),$$



which, together with the above estimate for the numerator of (3.30), proves (3.28). Notice that  $\prod_{i=j+1}^k \left(\frac{\sigma_i}{\sigma_j}\right)^2$  is always *bigger than one* for  $j = 1, 2, \dots, k-1$ . Therefore, for any  $k$ , combining (3.27) and (3.28) gives (3.29).  $\square$

REMARK 3.1. (3.27) and (3.29) have essentially been shown in [64]. Here we have given a general and complete proof. From (3.29), we get

$$(3.31) \quad (1 + \mathcal{O}(\rho^{-2})) |L_{k_1}^{(k)}(0)| = 1 + \mathcal{O}(\rho^{-2}), \quad k = 2, 3, \dots, n-1,$$

so the results in Theorem 3.1 are simplified as

$$(3.32) \quad \|\Delta_k\| \leq \frac{\sigma_{k+1}^{2+\beta}}{\sigma_k^{2+\beta}} (1 + \mathcal{O}(\rho^{-2})), \quad k = 1, 2, \dots, k_0,$$

$$(3.33) \quad \|\Delta_k\| \leq \frac{\sigma_{k+1}}{\sigma_k} (1 + \mathcal{O}(\rho^{-2})), \quad k = k_0 + 1, \dots, n-1.$$

REMARK 3.2. (3.28) illustrates that  $|L_j^{(k)}(0)|$  increases fast with  $j$  increasing and the smaller  $j$ , the smaller  $|L_j^{(k)}(0)|$ . (3.32) and (3.33) indicate that  $\mathcal{V}_k^R$  captures  $\mathcal{V}_k$  better for  $k \leq k_0$  than for  $k > k_0$ . That is, after the transition point  $k_0$ , the noise  $e$  starts to deteriorate  $\mathcal{V}_k^R$  and impairs its ability to capture  $\mathcal{V}_k$ .

In what follows we establish accurate estimates for  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  for moderately and mildly ill-posed problems.

THEOREM 3.3. Assume that (1.1) is moderately ill-posed with  $\sigma_j = \zeta j^{-\alpha}$ ,  $j = 1, 2, \dots, n$ , where  $\alpha > \frac{1}{2}$  and  $\zeta > 0$  is some constant, and the other assumptions and notation are the same as in Theorem 3.1. Then (3.3) holds with

$$(3.34) \quad \|\Delta_1\| \leq \frac{|u_2^T b|}{|u_1^T b|} \sqrt{\frac{1}{2\alpha - 1}},$$

$$(3.35) \quad \|\Delta_k\| \leq \frac{|u_{k+1}^T b|}{|u_k^T b|} \sqrt{\frac{k^2}{4\alpha^2 - 1} + \frac{k}{2\alpha - 1}} |L_{k_1}^{(k)}(0)|, \quad k = 2, 3, \dots, n-1.$$

Particularly, we have

$$(3.36) \quad \|\Delta_1\| \leq \frac{\sigma_2^{1+\beta}}{\sigma_1^{1+\beta}} \sqrt{\frac{1}{2\alpha - 1}},$$

$$(3.37) \quad \|\Delta_k\| \leq \frac{\sigma_{k+1}^{1+\beta}}{\sigma_k^{1+\beta}} \sqrt{\frac{k^2}{4\alpha^2 - 1} + \frac{k}{2\alpha - 1}} |L_{k_1}^{(k)}(0)|, \quad k = 2, 3, \dots, k_0,$$

$$(3.38) \quad \|\Delta_k\| \leq \sqrt{\frac{k^2}{4\alpha^2 - 1} + \frac{k}{2\alpha - 1}} |L_{k_1}^{(k)}(0)|, \quad k = k_0 + 1, \dots, n-1.$$

*Proof.* Following the proof of Theorem 3.1, we know that  $|\Delta_k| \leq |L_{k_1}^{(k)}(0)| \tilde{\Delta}_k$  still holds with  $\tilde{\Delta}_k$  defined by (3.18). So we only need to bound the right-hand side

of (3.19). For  $k = 1, 2, \dots, n-1$ , from (3.22) we get

$$\begin{aligned}
 \left( \sum_{j=k+1}^n \sigma_j^2 |u_j^T b|^2 \right)^{1/2} &= \sigma_{k+1} |u_{k+1}^T b| \left( \sum_{j=k+1}^n \frac{\sigma_j^2 |u_j^T b|^2}{\sigma_{k+1}^2 |u_{k+1}^T b|^2} \right)^{1/2} \\
 &\leq \sigma_{k+1} |u_{k+1}^T b| \left( \sum_{j=k+1}^n \frac{\sigma_j^2}{\sigma_{k+1}^2} \right)^{1/2} \\
 &= \sigma_{k+1} |u_{k+1}^T b| \left( \sum_{j=k+1}^n \left( \frac{j}{k+1} \right)^{-2\alpha} \right)^{1/2} \\
 &= \sigma_{k+1} |u_{k+1}^T b| \left( (k+1)^{2\alpha} \sum_{j=k+1}^n \frac{1}{j^{2\alpha}} \right)^{1/2} \\
 &< \sigma_{k+1} |u_{k+1}^T b| (k+1)^\alpha \left( \int_k^\infty \frac{1}{x^{2\alpha}} dx \right)^{1/2} \\
 &= \sigma_{k+1} |u_{k+1}^T b| \left( \frac{k+1}{k} \right)^\alpha \sqrt{\frac{k}{2\alpha-1}} \\
 &= \sigma_{k+1} |u_{k+1}^T b| \frac{\sigma_k}{\sigma_{k+1}} \sqrt{\frac{k}{2\alpha-1}} \\
 (3.39) \quad &= \sigma_k |u_{k+1}^T b| \sqrt{\frac{k}{2\alpha-1}}.
 \end{aligned}$$

Since the function  $x^{2\alpha}$  with any  $\alpha > \frac{1}{2}$  is convex over the interval  $[0, 1]$ , for  $k = 2, 3, \dots, n-1$ , from (3.22) we obtain

$$\begin{aligned}
 \left( \sum_{j=1}^k \frac{1}{\sigma_j^2 |u_j^T b|^2} \right)^{1/2} &= \frac{1}{\sigma_k |u_k^T b|} \left( \sum_{j=1}^k \frac{\sigma_k^2 |u_k^T b|^2}{\sigma_j^2 |u_j^T b|^2} \right)^{1/2} \leq \frac{1}{\sigma_k |u_k^T b|} \left( \sum_{j=1}^k \frac{\sigma_k^2}{\sigma_j^2} \right)^{1/2} \\
 &= \frac{1}{\sigma_k |u_k^T b|} \left( \sum_{j=1}^k \left( \frac{j}{k} \right)^{2\alpha} \right)^{1/2} \\
 (3.40) \quad &= \frac{1}{\sigma_k |u_k^T b|} \left( k \sum_{j=1}^k \frac{1}{k} \left( \frac{j-1}{k} \right)^{2\alpha} + 1 \right)^{1/2} \\
 &< \frac{1}{\sigma_k |u_k^T b|} \left( k \int_0^1 x^{2\alpha} dx + 1 \right)^{1/2} \\
 (3.41) \quad &= \frac{1}{\sigma_k |u_k^T b|} \sqrt{\frac{k}{2\alpha+1}} + 1.
 \end{aligned}$$

Substituting the above and (3.39) into (3.19) establishes (3.35), from which and (3.25), (3.26) it follows that (3.37) and (3.38) hold. For  $k = 1$ , we still have (3.24), from which and (3.39) we obtain (3.34). From (3.25) and (3.34) we get (3.36).  $\square$

REMARK 3.3. For a purely technical reason and for the sake of precise presentation, we have used the simplified singular value model  $\sigma_j = \zeta j^{-\alpha}$  to replace the general

form  $\sigma_j = \mathcal{O}(j^{-\alpha})$ , where the constant in each  $\mathcal{O}(\cdot)$  is implicit. This model, though simple, reflects the essence of moderately and mildly ill-posed problems and avoids some troublesome derivations and non-transparent formulations.

REMARK 3.4. In the spirit of the proof of Theorem 3.2, exploiting the first order Taylor expansion, we have an estimate

$$\begin{aligned}
 |L_{k_1}^{(k)}(0)| &\approx |L_k^{(k)}(0)| = \prod_{i=1}^{k-1} \frac{\sigma_i^2}{\sigma_i^2 - \sigma_k^2} = \prod_{i=1}^{k-1} \frac{1}{1 - \left(\frac{i}{k}\right)^{2\alpha}} \\
 &\approx 1 + \sum_{i=1}^{k-1} \left(\frac{i}{k}\right)^{2\alpha} = 1 + k \sum_{i=1}^k \frac{1}{k} \left(\frac{i-1}{k}\right)^{2\alpha} \\
 (3.42) \quad &< 1 + k \int_0^1 x^{2\alpha} dx = 1 + \frac{k}{2\alpha + 1},
 \end{aligned}$$

where the right-hand side of (3.42) increases linearly with respect to  $k$ .

REMARK 3.5. (3.34) and (3.36) indicate that  $\|\Delta_1\| < 1$  is guaranteed for moderately ill-posed problems with  $\alpha > 1$ . One might worry that the upper bounds (3.34) and (3.35) overestimate  $\|\Delta_k\|$  and thus  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  considerably because, in the proof, we have bounded the opaque  $\sum$  in (3.40) from above by the compact integral (3.41) nearest to it, which can be overestimates for  $k = 1, 2, \dots, k_0$ . It is not the case provided that  $k_0$  is not very small. In fact, since  $\alpha > \frac{1}{2}$ , we can bound (3.40) from below by the integral nearest to it:

$$\begin{aligned}
 \frac{1}{\sigma_k |u_k^T b|} \left( k \sum_{j=1}^k \frac{1}{k} \left(\frac{j-1}{k}\right)^{2\alpha} + 1 \right)^{1/2} &> \frac{1}{\sigma_k |u_k^T b|} \left( k \int_0^{\frac{k-1}{k}} x^{2\alpha} dx + 1 \right)^{1/2} \\
 &= \frac{1}{\sigma_k |u_k^T b|} \sqrt{\frac{k}{2\alpha + 1} \left(\frac{k-1}{k}\right)^{2\alpha+1} + 1},
 \end{aligned}$$

which is near to (3.41) once  $k \leq k_0$  is not very small. The smaller  $\alpha$ , the smaller the difference between the upper and lower bounds, i.e., the sharper (3.41).

REMARK 3.6. It is easily seen from (3.3) that  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  increases monotonically with respect to  $\|\Delta_k\|$ . For  $\|\Delta_k\|$  reasonably small and  $\|\Delta_k\|$  large we have

$$\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\| \approx \|\Delta_k\| \quad \text{and} \quad \|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\| \approx 1,$$

respectively. From (1.6) and (1.7), we obtain  $k_0 = \lfloor \eta^{-\frac{1}{\alpha(1+\beta)}} \rfloor - 1$ , where  $\lfloor \cdot \rfloor$  is the Gaussian function. For the white noise  $e$ , we have  $\eta \approx \frac{\|e\|}{\sqrt{m}}$ . As a result, for moderately ill-posed problems with  $\alpha > 1$ ,  $k_0$  is typically small and at most modest for a practical noise  $e$ , whose relative size  $\frac{\|e\|}{\|b\|}$  typically ranges from  $10^{-4}$  to  $10^{-2}$ . This means that for a moderately ill-posed problem  $\|\Delta_k\|$  is at most modest and cannot be large, so that  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\| < 1$  fairly.

REMARK 3.7. For severely ill-posed problems, since all the  $\frac{\sigma_{k+1}}{\sigma_k} \sim \rho^{-1}$ , a constant, (3.32) and (3.33) indicate that  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  is essentially unchanged for  $k = 1, 2, \dots, k_0$  and  $k = k_0 + 1, \dots, n - 1$ , respectively, that is,  $\mathcal{V}_k^R$  captures  $\mathcal{V}_k$  with almost the same accuracy for  $k \leq k_0$  and  $k > k_0$ , respectively. However, the situation is different for moderately ill-posed problems. For them,  $\frac{\sigma_{k+1}}{\sigma_k} = \left(\frac{k}{k+1}\right)^\alpha$  increases slowly as  $k$  increases, and the factor  $\sqrt{\frac{k^2}{4\alpha^2 - 1} + \frac{k}{2\alpha - 1}} |L_{k_1}^{(k)}(0)|$  increases as

$k$  grows. Therefore, (3.37) and (3.38) illustrate that  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  increases slowly with  $k \leq k_0$  and  $k > k_0$ , respectively. This means that  $\mathcal{V}_k^R$  may not capture  $\mathcal{V}_k$  so well as it does for severely ill-posed problems as  $k$  increases. In particular, starting with some  $k > k_0$ ,  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  starts to approach one, which indicates that, for  $k$  big,  $\mathcal{V}_k^R$  will contain substantial information on the right singular vectors corresponding to the  $n - k$  small singular values of  $A$ .

REMARK 3.8. For mildly ill-posed problems with  $\frac{1}{2} < \alpha \leq 1$ , there are some distinctive features. Note from (1.6) and (1.7) that  $k_0$  is now considerably bigger than that for a severely or moderately ill-posed problem with the same noise level  $\|e\|$  and  $\beta$ . As a result, firstly, for  $\alpha \leq 1$  and the same  $k$ , the factor  $\frac{\sigma_{k+1}}{\sigma_k} = \left(\frac{k}{k+1}\right)^\alpha$  is bigger than that for the moderately ill-posed problem; secondly,  $\sqrt{\frac{k^2}{4\alpha^2-1} + \frac{k}{2\alpha-1}} \sim k$  if  $\alpha \approx 1$  and is much bigger than  $k$  and can be arbitrarily large if  $\alpha \approx \frac{1}{2}$ ; thirdly, since  $\frac{1}{2} < \alpha \leq 1$ , for  $k \geq 3$  that ensures  $\frac{2\alpha+1}{k} \leq 1$ , we have

$$\begin{aligned}
 |L_{k_1}^{(k)}(0)| &\geq |L_k^{(k)}(0)| = \prod_{i=1}^{k-1} \frac{\sigma_i^2}{\sigma_i^2 - \sigma_k^2} = \prod_{i=1}^{k-1} \frac{1}{1 - \left(\frac{i}{k}\right)^{2\alpha}} \\
 &> 1 + \sum_{i=1}^{k-1} \left(\frac{i}{k}\right)^{2\alpha} > 1 + k \int_0^{\frac{k-1}{k}} x^{2\alpha} dx \\
 (3.43) \quad &= 1 + \frac{k \left(\frac{k-1}{k}\right)^{2\alpha+1}}{2\alpha+1} \approx 1 + \frac{k}{2\alpha+1} \left(1 - \frac{2\alpha+1}{k}\right) = \frac{k}{2\alpha+1},
 \end{aligned}$$

which also holds for moderately ill-posed problems and is bigger than one considerably for  $\frac{1}{2} < \alpha \leq 1$  as  $k$  increases up to  $k_0$ . Our accurate bound (3.37) thus becomes increasingly large as  $k$  increases up to  $k_0$  for mildly ill-posed problems, causing that  $\|\Delta_k\|$  is large and  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\| \approx 1$  starting with some  $k \leq k_0$ . Consequently,  $\mathcal{V}_{k_0}^R$  cannot effectively capture the  $k_0$  dominant right singular vectors and contains substantial information on the right singular vectors corresponding to the  $n - k_0$  small singular values.

REMARK 3.9. In [64, Thm 2.1], the authors derived some bounds for  $\|\Delta_k\|$  and  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$ . There, without realizing the crucial fact that  $|\Delta_k|$  can be effectively bounded by a rank one matrix and the key point that  $D_2 T_{k_2} T_{k_1}^{-1} D_1^{-1}$  must be treated as a whole other than separately, by (3.11) the authors made use of

$$\|\Delta_k\| \leq \|\Delta\|_F = \|D_2 T_{k_2} T_{k_1}^{-1} D_1^{-1}\|_F \leq \|D_2\| \|T_{k_2} T_{k_1}^{-1}\|_F \|D_1^{-1}\|$$

and  $\|T_{k_2} T_{k_1}^{-1}\|_F \leq |L_{k_1}^{(k)}(0)| \sqrt{k(n-k)}$  (cf. (3.16)) to obtain bounds for  $\|\Delta_k\|$  and  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$ . These bounds are too pessimistic because of the appearance of the fatal factor  $\sqrt{k(n-k)}$ , which ranges from  $\sqrt{2(n-2)}$  to  $\frac{n}{2}$  for  $k = 2, 3, \dots, n-1$ , too large amplification for  $n$  large. In contrast, our new estimates, which hold for both  $\|\Delta_k\|$  and  $\|\Delta_k\|_F$ , are much more accurate and  $\sqrt{k(n-k)}$  has been removed.

Before proceeding, we tentatively investigate how  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  affects the smallest Ritz value  $\theta_k^{(k)}$ . This problem is of central importance for understanding the regularizing effects of LSQR. We aim to lead the reader to a first manifestation that (i) we may have  $\theta_k^{(k)} > \sigma_{k+1}$  when  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\| < 1$  fairly, that is, no small Ritz value may appear provided that  $\mathcal{V}_k^R$  captures  $\mathcal{V}_k$  with only some other than high accuracy, and (ii) we must have  $\theta_k^{(k)} \leq \sigma_{k+1}$ , that is,  $\theta_k^{(k)}$  cannot approxi-

mate  $\sigma_k$  in natural order meaning that  $\theta_k^{(k)} \leq \sigma_{k_0+1}$  no later than iteration  $k_0$ , once  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  is sufficiently close to one.

**THEOREM 3.4.** *Let  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|^2 = 1 - \varepsilon_k^2$  with  $0 < \varepsilon_k < 1$ ,  $k = 1, 2, \dots, n-1$ , and let the unit-length  $\tilde{q}_k \in \mathcal{V}_k^R$  be a vector that has the smallest acute angle with  $\text{span}\{V_k^\perp\}$ , i.e., the closest to  $\text{span}\{V_k^\perp\}$ , where  $V_k^\perp$  is the matrix consisting of the last  $n-k$  columns of  $V$  defined by (1.4). Then it holds that*

$$(3.44) \quad \varepsilon_k^2 \sigma_k^2 + (1 - \varepsilon_k^2) \sigma_n^2 < \tilde{q}_k^T A^T A \tilde{q}_k < \varepsilon_k^2 \sigma_{k+1}^2 + (1 - \varepsilon_k^2) \sigma_1^2.$$

If  $\varepsilon_k \geq \frac{\sigma_{k+1}}{\sigma_k}$ , then

$$(3.45) \quad \sqrt{\tilde{q}_k^T A^T A \tilde{q}_k} > \sigma_{k+1};$$

if  $\varepsilon_k^2 \leq \frac{\delta}{(\frac{\sigma_1}{\sigma_{k+1}})^2 - 1}$  for a given arbitrarily small  $\delta > 0$ , then

$$(3.46) \quad \theta_k^{(k)} < (1 + \delta)^{1/2} \sigma_{k+1}.$$

*Proof.* Since the columns of  $Q_k$  generated by Lanczos bidiagonalization form an orthonormal basis of  $\mathcal{V}_k^R$ , by definition and the assumption on  $\tilde{q}_k$  we have

$$\begin{aligned} \|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\| &= \|(V_k^\perp)^T Q_k\| = \|V_k^\perp (V_k^\perp)^T Q_k\| \\ &= \max_{\|c\|=1} \|V_k^\perp (V_k^\perp)^T Q_k c\| = \|V_k^\perp (V_k^\perp)^T Q_k c_k\| \\ (3.47) \quad &= \|V_k^\perp (V_k^\perp)^T \tilde{q}_k\| = \|(V_k^\perp)^T \tilde{q}_k\| = \sqrt{1 - \varepsilon_k^2} \end{aligned}$$

with  $\tilde{q}_k = Q_k c_k \in \mathcal{V}_k^R$  and  $\|c_k\| = 1$ . Since  $\mathcal{V}_k$  is the orthogonal complement of  $\text{span}\{V_k^\perp\}$ , by definition we know that  $\tilde{q}_k \in \mathcal{V}_k^R$  has the largest acute angle with  $\mathcal{V}_k$ , that is, it is the vector in  $\mathcal{V}_k^R$  that contains the least information on  $\mathcal{V}_k$ .

Expand  $\tilde{q}_k$  as the following orthogonal direct sum decomposition:

$$(3.48) \quad \tilde{q}_k = V_k^\perp (V_k^\perp)^T \tilde{q}_k + V_k V_k^T \tilde{q}_k.$$

Then from  $\|\tilde{q}_k\| = 1$  and (3.47) we obtain

$$(3.49) \quad \|V_k^T \tilde{q}_k\| = \|V_k V_k^T \tilde{q}_k\| = \sqrt{1 - \|(V_k^\perp)^T \tilde{q}_k\|^2} = \sqrt{1 - (1 - \varepsilon_k^2)} = \varepsilon_k.$$

From (3.48), we next bound the Rayleigh quotient of  $\tilde{q}_k$  with respect to  $A^T A$  from below. By the SVD (1.4) of  $A$  and  $V = (V_k, V_k^\perp)$ , we partition

$$\Sigma = \begin{pmatrix} \Sigma_k & \\ & \Sigma_k^\perp \end{pmatrix},$$

where  $\Sigma_k = \text{diag}(\sigma_1, \sigma_2, \dots, \sigma_k)$  and  $\Sigma_k^\perp = \text{diag}(\sigma_{k+1}, \sigma_{k+2}, \dots, \sigma_n)$ . Making use of  $A^T A V_k = V_k \Sigma_k^2$  and  $A^T A V_k^\perp = V_k^\perp (\Sigma_k^\perp)^2$  as well as  $V_k^T V_k^\perp = \mathbf{0}$ , we obtain

$$\begin{aligned} \tilde{q}_k^T A^T A \tilde{q}_k &= (V_k^\perp (V_k^\perp)^T \tilde{q}_k + V_k V_k^T \tilde{q}_k)^T A^T A (V_k^\perp (V_k^\perp)^T \tilde{q}_k + V_k V_k^T \tilde{q}_k) \\ &= (\tilde{q}_k^T V_k^\perp (V_k^\perp)^T + \tilde{q}_k^T V_k V_k^T) (V_k^\perp (\Sigma_k^\perp)^2 (V_k^\perp)^T \tilde{q}_k + V_k \Sigma_k^2 V_k^T \tilde{q}_k) \\ (3.50) \quad &= \tilde{q}_k^T V_k^\perp (\Sigma_k^\perp)^2 (V_k^\perp)^T \tilde{q}_k + \tilde{q}_k^T V_k \Sigma_k^2 V_k^T \tilde{q}_k. \end{aligned}$$

Observe that it is impossible for  $(V_k^\perp)^T \tilde{q}_k$  and  $V_k^T \tilde{q}_k$  to be the eigenvectors of  $(\Sigma_k^\perp)^2$  and  $\Sigma_k^2$  associated with their respective smallest eigenvalues  $\sigma_n^2$  and  $\sigma_k^2$  simultaneously, which are the  $(n-k)$ -th canonical vector  $e_{n-k}$  of  $\mathbb{R}^{n-k}$  and the  $k$ -th canonical vector  $e_k$  of  $\mathbb{R}^k$ , respectively; otherwise, we have  $\tilde{q}_k = v_n$  and  $\tilde{q}_k = v_k$  simultaneously, which are impossible as  $k < n$ . Therefore, from (3.50) and (3.47), (3.49) we obtain the strict inequality

$$\tilde{q}_k^T A^T A \tilde{q}_k > \|(V_k^\perp)^T \tilde{q}_k\|^2 \sigma_n^2 + \|V_k^T \tilde{q}_k\|^2 \sigma_k^2 = (1 - \varepsilon_k^2) \sigma_n^2 + \varepsilon_k^2 \sigma_k^2,$$

from which it follows that the lower bound of (3.44) holds. Similarly, from (3.50) and (3.47), (3.49) we obtain the upper bound of (3.44):

$$\tilde{q}_k^T A^T A \tilde{q}_k < \|(V_k^\perp)^T \tilde{q}_k\|^2 \|\Sigma_k^\perp\|^2 + \|V_k^T \tilde{q}_k\|^2 \|\Sigma_k\|^2 = (1 - \varepsilon_k^2) \sigma_{k+1}^2 + \varepsilon_k^2 \sigma_1^2.$$

From the lower bound of (3.44), we see that if  $\varepsilon_k$  satisfies  $\varepsilon_k^2 \sigma_k^2 \geq \sigma_{k+1}^2$ , i.e.,  $\varepsilon_k \geq \frac{\sigma_{k+1}}{\sigma_k}$ , then  $\sqrt{\tilde{q}_k^T A^T A \tilde{q}_k} > \sigma_{k+1}$ , i.e., (3.45) holds.

From (2.4), we obtain  $B_k^T B_k = Q_k^T A^T A Q_k$ . Note that  $(\theta_k^{(k)})^2$  is the smallest eigenvalue of the symmetric positive definite matrix  $B_k^T B_k$ . Therefore, we have

$$(3.51) \quad (\theta_k^{(k)})^2 = \min_{\|c\|=1} c^T Q_k^T A^T A Q_k c = \min_{q \in \mathcal{V}_k^R, \|q\|=1} q^T A^T A q = \hat{q}_k^T A^T A \hat{q}_k,$$

where  $\hat{q}_k$  is, in fact, the Ritz vector of  $A^T A$  from  $\mathcal{V}_k^R$  corresponding to the smallest Ritz value  $(\theta_k^{(k)})^2$ . Therefore, for  $\tilde{q}_k$  defined in Theorem 3.4 we have

$$\theta_k^{(k)} \leq \sqrt{\tilde{q}_k^T A^T A \tilde{q}_k},$$

from which it follows from (3.44) that  $(\theta_k^{(k)})^2 < (1 - \varepsilon_k^2) \sigma_{k+1}^2 + \varepsilon_k^2 \sigma_1^2$ . As a result, for any  $\delta > 0$ , we can choose  $\varepsilon_k \geq 0$  such that

$$(\theta_k^{(k)})^2 < (1 - \varepsilon_k^2) \sigma_{k+1}^2 + \varepsilon_k^2 \sigma_1^2 \leq (1 + \delta) \sigma_{k+1}^2,$$

i.e., (3.46) holds, solving which for  $\varepsilon_k^2$  gives  $\varepsilon_k^2 \leq \frac{\delta}{(\frac{\sigma_1}{\sigma_{k+1}})^2 - 1}$ .  $\square$

**REMARK 3.10.** We analyze  $\theta_k^{(k)}$  for  $\varepsilon_k \geq \frac{\sigma_{k+1}}{\sigma_k}$ . A key observation and interpretation is that, in the sense of  $\min$  in (3.51),  $\hat{q}_k \in \mathcal{V}_k^R$  is the optimal vector that extracts the least information from  $\mathcal{V}_k$  and the richest information from  $\text{span}\{V_k^\perp\}$ . From Theorem 3.4, since  $\mathcal{V}_k$  is the orthogonal complement of  $\text{span}\{V_k^\perp\}$ , we know that  $\tilde{q}_k \in \mathcal{V}_k^R$  has the largest acute angle with  $\mathcal{V}_k$ , that is, it contains the least information from  $\mathcal{V}_k$  and the richest information from  $\text{span}\{V_k^\perp\}$ . Therefore,  $\hat{q}_k$  and  $\tilde{q}_k$  have a similar optimality, so that we have

$$(3.52) \quad \theta_k^{(k)} \approx \sqrt{\tilde{q}_k^T A^T A \tilde{q}_k}.$$

Combining this estimate with (3.45), we may have  $\theta_k^{(k)} > \sigma_{k+1}$  when  $\varepsilon_k \geq \frac{\sigma_{k+1}}{\sigma_k}$ .

**REMARK 3.11.** We inspect the condition  $\varepsilon_k \geq \frac{\sigma_{k+1}}{\sigma_k}$  for (3.45) and get insight into whether or not the true  $\varepsilon_k$  resulting from three kinds of ill-posed problems satisfies it. For severely ill-posed problems, the lower bound  $\frac{\sigma_{k+1}}{\sigma_k}$  is basically the constant  $\rho^{-1}$ ; for moderately ill-posed problems with  $\alpha > 1$ , the bound increases with increasing  $k \leq k_0$ , and it cannot be close to one provided that  $\alpha > 1$  suitably or  $k_0$  not big;



for mildly ill-posed problems with  $\alpha < 1$ , the bound increases faster than it does for moderately ill-posed problems, and it may well approach one for  $k \leq k_0$ . Therefore, the condition for (3.45) requires that  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  be not close to one for severely and moderately ill-posed problems, but  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  must be close to zero for mildly ill-posed problems. In view of (3.3) and  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|^2 = 1 - \varepsilon_k^2$ , we have  $\|\Delta_k\|^2 = \frac{1 - \varepsilon_k^2}{\varepsilon_k^2}$ . Thus, the condition  $\varepsilon_k \geq \frac{\sigma_{k+1}}{\sigma_k}$  for (3.45) amounts to requiring that  $\|\Delta_k\|$  be at most modest and cannot be large for severely and moderately ill-posed problems but it must be fairly small for mildly ill-posed problems. Unfortunately, Theorems 3.1–3.3 and the remarks followed indicate that  $\|\Delta_k\|$  increases with  $k$  increasing and is generally large for a mildly ill-posed problem, while it increases slowly with  $k \leq k_0$  for a moderately ill-posed problem with  $\alpha > 1$  suitably, and by (3.32) it is approximately a constant  $\rho^{-(2+\beta)}$ , which is smaller than one considerably for a severely ill-posed problem with  $\rho > 1$  not close to one. Consequently, for mildly ill-posed problems, because the actual  $\|\Delta_k\|$  can hardly be small and is generally large, the true  $\varepsilon_k$  is small and may well be close to one, so that the condition  $\varepsilon_k \geq \frac{\sigma_{k+1}}{\sigma_k}$  generally fails to meet as  $k$  increases, while it is satisfied for severely or moderately ill-posed problems with  $\rho > 1$  or  $\alpha > 1$  suitably.

REMARK 3.12. (3.46) shows that there is at least one Ritz value  $\theta_k^{(k)} \leq \sigma_{k+1}$  when  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  is sufficiently close to one since we can choose  $\delta$  small enough such that  $(1 + \delta)^{1/2} \sigma_{k+1}$  is close to  $\sigma_{k+1}$  arbitrarily. As we have shown,  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  cannot be close to one for severely or moderately ill-posed problems with  $\rho > 1$  or  $\alpha > 1$  suitably, but it is generally so for mildly ill-posed problems. This means that for some  $k \leq k_0$  it is very possible to have  $\theta_k^{(k)} \leq \sigma_{k+1}$  for mildly ill-posed problems.

We must be aware that our above analysis on  $\theta_k^{(k)} > \sigma_{k+1}$  is not rigorous because we cannot quantify how small  $\sqrt{\tilde{q}_k^T A^T A \tilde{q}_k} - \theta_k^{(k)}$  is. From  $\theta_k^{(k)} \leq \sqrt{\tilde{q}_k^T A^T A \tilde{q}_k}$ , it is apparent that the condition  $\varepsilon_k \geq \frac{\sigma_{k+1}}{\sigma_k}$  may not be sufficient for  $\theta_k^{(k)} > \sigma_{k+1}$  though it is so for  $\sqrt{\tilde{q}_k^T A^T A \tilde{q}_k} > \sigma_{k+1}$ . We delay our detailed and rigorous analysis to Section 4, where we present a number of deep-going and accurate results on the key problems stated in the last second paragraph before Theorem 3.1, including the precise behavior of  $\theta_k^{(k)}$ . One of the results will be on the sufficient conditions for  $\theta_k^{(k)} > \sigma_{k+1}$ , which are satisfied when certain deterministic and mild restrictions on  $\rho$  or  $\alpha$  are imposed for severely or moderately ill-posed problems. However, we will see that  $\alpha < 1$  for mildly ill-posed problems never meets the sufficient conditions to be presented there.

Theorems 3.1–3.3 establish necessary background for answering the fundamental concern by Björck and Eldén, and their proof approaches also provide key ingredients for some of the later results. We next present the following results, which will play a central role in our later analysis.

THEOREM 3.5. Assume that the discrete Picard condition (1.6) is satisfied, let  $\Delta_k \in \mathbb{R}^{(n-k) \times k}$  be defined as (3.11) and  $L_j^{(k)}(0)$  and  $L_{k_1}^{(k)}(0)$  be defined as (3.6), and write  $\Delta_k = (\delta_1, \delta_2, \dots, \delta_k)$ . Then for severely ill-posed problems and  $k = 1, 2, \dots, n-1$  we have

$$(3.53) \quad \|\delta_j\| \leq \frac{\sigma_{k+1}}{\sigma_j} \frac{|u_{k+1}^T b|}{|u_j^T b|} (1 + \mathcal{O}(\rho^{-2})) |L_j^{(k)}(0)|, \quad k > 1, \quad j = 1, 2, \dots, k,$$

$$(3.54) \quad \|\delta_1\| \leq \frac{\sigma_2}{\sigma_1} \frac{|u_2^T b|}{|u_1^T b|} (1 + \mathcal{O}(\rho^{-2})) |L_1^{(k)}(0)|, \quad k = 1$$

and

$$(3.55) \quad \|\Sigma_k \Delta_k^T\| \leq \begin{cases} \sigma_{k+1} \frac{|u_{k+1}^T b|}{|u_k^T b|} (1 + \mathcal{O}(\rho^{-2})) & \text{for } 1 \leq k \leq k_0, \\ \sigma_{k+1} \sqrt{k - k_0 + 1} (1 + \mathcal{O}(\rho^{-2})) & \text{for } k_0 < k \leq n-1; \end{cases}$$

for moderately or mild ill-posed problems with the singular values  $\sigma_j = \zeta j^{-\alpha}$  and  $\zeta$  a positive constant we have

$$(3.56) \quad \|\delta_j\| \leq \frac{\sigma_k}{\sigma_j} \frac{|u_{k+1}^T b|}{|u_j^T b|} \sqrt{\frac{k}{2\alpha-1}} |L_j^{(k)}(0)|, \quad k > 1, \quad j = 1, 2, \dots, k,$$

$$(3.57) \quad \|\delta_1\| \leq \frac{|u_2^T b|}{|u_1^T b|} \sqrt{\frac{1}{2\alpha-1}}, \quad k = 1$$

and

$$(3.58) \quad \|\Sigma_k \Delta_k^T\| \leq \begin{cases} \sigma_1 \frac{|u_2^T b|}{|u_1^T b|} \sqrt{\frac{1}{2\alpha-1}} & \text{for } k = 1, \\ \sigma_k \frac{|u_{k+1}^T b|}{|u_k^T b|} \sqrt{\frac{k^2}{4\alpha^2-1} + \frac{k}{2\alpha-1}} |L_{k_1}^{(k)}(0)| & \text{for } 1 < k \leq k_0, \\ \sigma_k \sqrt{\frac{k k_0}{4\alpha^2-1} + \frac{k(k-k_0+1)}{2\alpha-1}} |L_{k_1}^{(k)}(0)| & \text{for } k_0 < k \leq n-1. \end{cases}$$

*Proof.* From (3.11) and (3.17), for  $j = 1, 2, \dots, k$  and  $k > 1$  we have

$$(3.59) \quad \|\delta_j\|^2 \leq |L_j^{(k)}(0)|^2 \sum_{i=k+1}^n \frac{\sigma_i^2 |u_i^T b|^2}{\sigma_j^2 |u_j^T b|^2}$$

and from (3.24), for  $k = 1$  we have

$$(3.60) \quad \|\delta_1\|^2 = \sum_{i=2}^n \frac{\sigma_i^2 |u_i^T b|^2}{\sigma_1^2 |u_1^T b|^2}.$$

For severely ill-posed problems,  $k = 1, 2, \dots, n-1$  and  $j = 1, 2, \dots, k$ , from (3.23) we obtain

$$\begin{aligned} \sum_{i=k+1}^n \frac{\sigma_i^2 |u_i^T b|^2}{\sigma_j^2 |u_j^T b|^2} &= \frac{1}{\sigma_j^2 |u_j^T b|^2} \sum_{i=k+1}^n \sigma_i^2 |u_i^T b|^2 \\ &\leq \frac{\sigma_{k+1}^2 |u_{k+1}^T b|^2}{\sigma_j^2 |u_j^T b|^2} (1 + \mathcal{O}(\rho^{-2})). \end{aligned}$$

For moderately or mildly ill-posed problems,  $k = 1, 2, \dots, n-1$  and  $j = 1, 2, \dots, k$ , from (3.39) we obtain

$$\begin{aligned} \sum_{i=k+1}^n \frac{\sigma_i^2 |u_i^T b|^2}{\sigma_j^2 |u_j^T b|^2} &= \frac{1}{\sigma_j^2 |u_j^T b|^2} \sum_{i=k+1}^n \sigma_i^2 |u_i^T b|^2 \\ &\leq \frac{\sigma_k^2 |u_{k+1}^T b|^2}{\sigma_j^2 |u_j^T b|^2} \frac{k}{2\alpha-1}. \end{aligned}$$

Combining the above with (3.59), (3.29) and (3.31), we obtain (3.53), while (3.56) follows from the above and (3.59) directly. For  $k = 1$ , from (3.60) and the above we get (3.54) and (3.57), respectively.

By (3.18), for  $k > 1$  we have

$$|\Delta_k \Sigma_k| \leq |L_{k_1}^{(k)}(0)| \left| (\sigma_{k+1} u_{k+1}^T b, \sigma_{k+2} u_{k+2}^T b, \dots, \sigma_n u_n^T b)^T \left( \frac{1}{u_1^T b}, \frac{1}{u_2^T b}, \dots, \frac{1}{u_k^T b} \right) \right|.$$

Therefore, we get

$$(3.61) \quad \begin{aligned} \|\Sigma_k \Delta_k^T\| &= \|\Delta_k \Sigma_k\| \leq \|\Delta_k \Sigma_k\| \\ &\leq |L_{k_1}^{(k)}(0)| \left( \sum_{j=k+1}^n \sigma_j^2 |u_j^T b|^2 \right)^{1/2} \left( \sum_{j=1}^k \frac{1}{|u_j^T b|^2} \right)^{1/2}. \end{aligned}$$

By (3.24), for  $k = 1$  we have

$$\|\Delta_1 \Sigma_1\| = \left( \sum_{j=2}^n \sigma_j^2 |u_j^T b|^2 \right)^{1/2} \frac{1}{|u_1^T b|}.$$

We have derived the bounds (3.23) and (3.39) for  $\left( \sum_{j=k+1}^n \sigma_j^2 |u_j^T b|^2 \right)^{1/2}$  for severely and moderately or mildly ill-posed problems, respectively, from which we obtain (3.55) and (3.58) for  $k = 1$ . In order to bound  $\|\Sigma_k \Delta_k^T\|$  for  $k > 1$ , we need to estimate  $\left( \sum_{j=1}^k \frac{1}{|u_j^T b|^2} \right)^{1/2}$ . We next carry out this task for severely and moderately or mildly ill-posed problems, respectively, for each kind of which we consider the cases of  $k \leq k_0$  and  $k > k_0$  separately.

Case of  $k \leq k_0$  for severely ill-posed problems: From the discrete Picard condition (1.6) and (3.20), we obtain

$$\begin{aligned} \sum_{j=1}^k \frac{1}{|u_j^T b|^2} &= \frac{1}{|u_k^T b|^2} \sum_{j=1}^k \frac{|u_k^T b|^2}{|u_j^T b|^2} = \frac{1}{|u_k^T b|^2} \left( 1 + \mathcal{O} \left( \sum_{j=1}^{k-1} \rho^{2(j-k)(1+\beta)} \right) \right) \\ &= \frac{1}{|u_k^T b|^2} \left( 1 + \mathcal{O}(\rho^{-2(1+\beta)}) \right). \end{aligned}$$

Case of  $k > k_0$  for severely ill-posed problems: From (3.20) and (3.21), we obtain

$$\begin{aligned} \sum_{j=1}^k \frac{1}{|u_j^T b|^2} &= \frac{1}{|u_k^T b|^2} \left( \sum_{j=1}^{k_0} \frac{|u_k^T b|^2}{|u_j^T b|^2} + \sum_{j=k_0+1}^k \frac{|u_k^T b|^2}{|u_j^T b|^2} \right) \\ &= \frac{1}{|u_k^T b|^2} \left( 1 + \mathcal{O} \left( \sum_{j=1}^{k_0-1} \rho^{2(j-k_0)(1+\beta)} \right) + k - k_0 \right) \\ &= \frac{1}{|u_k^T b|^2} \left( 1 + \mathcal{O}(\rho^{-2(1+\beta)}) + k - k_0 \right). \end{aligned}$$

Substituting the above two relations for the two cases into (3.61) and combining them with (3.23) and (3.29), we get (3.55).

Case of  $k \leq k_0$  for moderately or mildly ill-posed problems: From (3.20) we have

$$\begin{aligned} \sum_{j=1}^k \frac{1}{|u_j^T b|^2} &= \frac{1}{|u_k^T b|^2} \sum_{j=1}^k \frac{|u_k^T b|^2}{|u_j^T b|^2} = \frac{1}{|u_k^T b|^2} \sum_{j=1}^k \left(\frac{j}{k}\right)^{2\alpha(1+\beta)} \\ &< \frac{1}{|u_k^T b|^2} \sum_{j=1}^k \left(\frac{j}{k}\right)^{2\alpha} = \frac{1}{|u_k^T b|^2} k \sum_{j=1}^k \frac{1}{k} \left(\frac{j}{k}\right)^{2\alpha} \\ &< \frac{1}{|u_k^T b|^2} \left( k \int_0^1 x^{2\alpha} dx + 1 \right) = \frac{1}{|u_k^T b|^2} \left( \frac{k}{2\alpha+1} + 1 \right). \end{aligned}$$

Case of  $k > k_0$  for moderately or mildly ill-posed problems: From (3.20) and (3.21) we have

$$\begin{aligned} \sum_{j=1}^k \frac{1}{|u_j^T b|^2} &= \frac{1}{|u_k^T b|^2} \left( \sum_{j=1}^{k_0} \frac{|u_k^T b|^2}{|u_j^T b|^2} + \sum_{j=k_0+1}^k \frac{|u_k^T b|^2}{|u_j^T b|^2} \right) \\ &= \frac{1}{|u_k^T b|^2} \left( \sum_{j=1}^{k_0} \left(\frac{j}{k_0}\right)^{2\alpha(1+\beta)} + k - k_0 \right) \\ &< \frac{1}{|u_k^T b|^2} \left( \sum_{j=1}^{k_0} \left(\frac{j}{k_0}\right)^{2\alpha} + k - k_0 \right) \\ &\leq \frac{1}{|u_k^T b|^2} \left( \frac{k_0}{2\alpha+1} + 1 + k - k_0 \right). \end{aligned}$$

Substituting the above two bounds for the two cases into (3.61) and combining them with (3.39), we get (3.58).  $\square$

(3.55) and (3.58) indicate that  $\|\Sigma_k \Delta_k^T\|$  decays swiftly as  $k$  increases. As has been seen, we must take some cares to accurately bound  $\|\Sigma_k \Delta_k^T\|$ . Indeed, for  $1 < k \leq k_0$ , if we had simply bounded it by

$$(3.62) \quad \|\Sigma_k \Delta_k^T\| \leq \|\Sigma_k\| \|\Delta_k^T\| = \sigma_1 \|\Delta_k\|,$$

the factors  $\sigma_{k+1}$  in (3.55) and  $\sigma_k$  in (3.58) would have been replaced by  $\frac{\sigma_1 \sigma_{k+1}}{\sigma_k} \approx \sigma_1 \rho^{-1}$  and  $\sigma_1$ , respectively, by substituting the estimates (3.5) and (3.35) for  $\|\Delta_k\|$  into the above. Such bounds overestimate  $\|\Sigma_k \Delta_k^T\|$  too much as  $k$  increases, and are useless to precisely analyze the regularization of LSQR, CGME and LSMR for ill-posed problems since they make us impossible to get those predictively accurate results to be presented in Sections 4–6.

As a byproduct, we consider an interesting problem that has its own right, though its solution will not be used in this paper: How close to the Krylov subspace  $\mathcal{V}_k^R$  is the individual right singular vector  $v_j$  for  $j \leq k$  and  $k = 1, 2, \dots, n-1$ ? Denote by  $\sin \angle(v_j, \mathcal{V}_k^R)$  the distance between  $v_j$  and  $\mathcal{V}_k^R$ , which is defined as

$$\sin \angle(v_j, \mathcal{V}_k^R) = \|(I - \Pi_k)v_j\| = \min_{w \in \mathcal{V}_k^R} \|v_j - w\|$$

with  $\Pi_k$  the orthogonal projector onto  $\mathcal{V}_k^R$ . Then we present the following result.

**THEOREM 3.6.** *Let  $\Delta_k = (\delta_1, \delta_2, \dots, \delta_k)$  be defined by (3.11). Then for  $k =$*

$1, 2, \dots, n-1$  and  $j = 1, 2, \dots, k$  we have

$$(3.63) \quad \frac{\sigma_{\min}(\Delta_k)}{\sqrt{1 + \sigma_{\min}^2(\Delta_k)}} \leq \sin \angle(v_j, \mathcal{V}_k^R) \leq \min\{\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|, \|\delta_j\|\},$$

where  $\sigma_{\min}(\cdot)$  denotes the smallest singular value of a matrix.

*Proof.* We first prove the upper bound of (3.63). Since the columns of  $Z_k$  defined by (3.12) form a basis of  $\mathcal{V}_k^R$ , its  $j$ -th column  $Z_k e_j \in \mathcal{V}_k^R$ . As a result, we get

$$\begin{aligned} \sin \angle(v_j, \mathcal{V}_k^R) &= \min_{w \in \mathcal{V}_k^R} \|v_j - w\| \leq \|v_j - Z_k e_j\| \\ &= \|v_j - (V_k + V_k^\perp \Delta_k) e_j\| = \|v_j - v_j - V_k^\perp \delta_j\| \\ &= \|V_k^\perp \delta_j\| = \|\delta_j\|. \end{aligned}$$

Recall from (3.13) that the columns of  $\hat{Z}_k$  form an orthonormal basis of  $\mathcal{V}_k^R$ , and suppose that  $(\hat{Z}_k, \hat{Z}_k^\perp)$  is orthogonal. Then the columns of  $\hat{Z}_k^\perp$  are an orthonormal basis of the orthogonal complement of  $\mathcal{V}_k^R$  with respect to  $\mathbb{R}^n$ . Particularly,

$$\hat{Z}_k^\perp = (V_k^\perp - V_k \Delta_k^T)(I + \Delta_k \Delta_k^T)^{-\frac{1}{2}}$$

meets the requirement. By definition, we obtain

$$\begin{aligned} \|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\| &= \|(\hat{Z}_k^\perp)^T V_k\| = \|\hat{Z}_k^\perp (\hat{Z}_k^\perp)^T V_k\| = \max_{\|c\|=1} \|\hat{Z}_k^\perp (\hat{Z}_k^\perp)^T V_k c\| \\ &= \max_{\|c\|=1} \|(I - \hat{Z}_k \hat{Z}_k^T) V_k c\| = \max_{\|c\|=1} \|(I - \Pi_k) V_k c\|, \end{aligned}$$

from which and  $v_j = V_k e_j$  it follows that

$$\sin \angle(v_j, \mathcal{V}_k^R) \leq \|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$$

by taking  $c = e_j$ ,  $j = 1, 2, \dots, k$ . So the upper bound of (3.63) holds.

We next derive the lower bound of (3.63). We obtain from above that

$$\begin{aligned} \sin \angle(v_j, \mathcal{V}_k^R) &= \|(I - \Pi_k) v_j\| = \|(\hat{Z}_k^\perp)^T v_j\| \\ &= \|(I + \Delta_k \Delta_k^T)^{-\frac{1}{2}} ((V_k^\perp)^T - \Delta_k V_k^T) v_j\| \\ &= \|(I + \Delta_k \Delta_k^T)^{-\frac{1}{2}} \Delta_k e_j\| \\ &\geq \sigma_{\min} \left( (I + \Delta_k \Delta_k^T)^{-\frac{1}{2}} \Delta_k \right) = \frac{\sigma_{\min}(\Delta_k)}{\sqrt{1 + \sigma_{\min}^2(\Delta_k)}}. \quad \square \end{aligned}$$

We remark that the lower bound in (3.63) is just the sine of the smallest canonical angle of  $\mathcal{V}_k$  and  $\mathcal{V}_k^R$ . Since  $v_j \in \mathcal{V}_k$ , it is natural that  $\angle(v_j, \mathcal{V}_k^R)$  lies between the smallest and largest angles of  $\mathcal{V}_k$  and  $\mathcal{V}_k^R$ , as (3.63) indicates. The nontrivial point of the upper bound in (3.63) is that  $\sin \angle(v_j, \mathcal{V}_k^R)$  can be much smaller than  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$ , as indicated by the bounds (3.53) and (3.56), especially for  $j$  not close to  $k$ . Combining (3.63) with (3.53) and (3.56), we see that the smaller  $j$ , the closer  $v_j$  is to  $\mathcal{V}_k^R$ .

**4. The rank  $k$  approximation  $P_{k+1}B_kQ_k^T$  to  $A$ , the Ritz values  $\theta_i^{(k)}$  and the regularization of LSQR.** Making use of Theorems 3.1–3.5, we are able to solve those key problems stated before Theorem 3.1 and give definitive answers to the fundamental concern by Björck and Eldén, proving that LSQR has the full regularization for severely or moderately ill-posed problems with  $\rho > 1$  or  $\alpha > 1$  suitably and it, in general, has only the partial regularization for mildly ill-posed problems.

Define

$$(4.1) \quad \gamma_k = \|A - P_{k+1}B_kQ_k^T\|,$$

which measures the accuracy of the rank  $k$  approximation  $P_{k+1}B_kQ_k^T$  to  $A$  generated by Lanczos bidiagonalization. Recall (2.6) and the comments followed. It is known that the full or partial regularization of LSQR uniquely depends on whether or not  $\gamma_k \approx \sigma_{k+1}$  holds, where we will make the precise meaning ‘ $\approx$ ’ clear by introducing the definition of near best rank  $k$  approximation to  $A$ , and on whether or not the  $k$  singular values  $\theta_i^{(k)}$ , i.e., Ritz values, of  $B_k$ , approximate the  $k$  large singular values  $\sigma_i$  of  $A$  in natural order for  $k = 1, 2, \dots, k_0$ . If both of them hold, LSQR has the full regularization; if either of them is not satisfied, LSQR has only the partial regularization.

This section consists of three subsections. In Section 4.1, we present accurate estimates for  $\gamma_k$  for the three kinds of ill-posed problems under consideration. We prove that, under some reasonable conditions on  $\rho$  or  $\alpha$ , the matrix  $P_{k+1}B_kQ_k^T$  is a near best rank  $k$  approximation to  $A$ . In Section 4.2, we deepen the results in Section 4.1 and show how the  $k$  Ritz values  $\theta_i^{(k)}$  behave. We derive the sufficient conditions on  $\rho$  and  $\alpha$  for which they approximate the first  $k$  large singular values  $\sigma_i$  of  $A$  in natural order. In Section 4.3, we consider general best and near best rank approximations to  $A$  with respect to the 2-norm. For  $A$  with  $\sigma_i = \zeta i^{-\alpha}$ ,  $i = 1, 2, \dots, n$ , we analyze the nonzero singular values of such a rank  $k$  approximation, and prove that they approximate the first  $k$  large singular values of  $A$  for  $\alpha > 1$  suitably but can fail to do so for  $\frac{1}{2} < \alpha \leq 1$ . These results will help understand the regularizing effects of LSQR.

**4.1. The accuracy of rank  $k$  approximation  $P_{k+1}B_kQ_k^T$  to  $A$  and more related.** We first present one of the main results in this paper.

**THEOREM 4.1.** *Assume that the discrete Picard condition (1.6) is satisfied. Then for  $k = 1, 2, \dots, n-1$  we have*

$$(4.2) \quad \sigma_{k+1} \leq \gamma_k \leq \sqrt{1 + \eta_k^2} \sigma_{k+1}$$

with

$$(4.3) \quad \eta_k \leq \begin{cases} \xi_k \frac{|u_{k+1}^T b|}{|u_k^T b|} (1 + \mathcal{O}(\rho^{-2})) & \text{for } 1 \leq k \leq k_0, \\ \xi_k \sqrt{k - k_0 + 1} (1 + \mathcal{O}(\rho^{-2})) & \text{for } k_0 < k \leq n-1 \end{cases}$$

for severely ill-posed problems and

$$(4.4) \quad \eta_k \leq \begin{cases} \xi_1 \frac{\sigma_1}{\sigma_2} \frac{|u_2^T b|}{|u_1^T b|} \sqrt{\frac{1}{2\alpha-1}} & \text{for } k = 1, \\ \xi_k \frac{\sigma_k}{\sigma_{k+1}} \frac{|u_{k+1}^T b|}{|u_k^T b|} \sqrt{\frac{k^2}{4\alpha^2-1} + \frac{k}{2\alpha-1}} |L_{k_1}^{(k)}(0)| & \text{for } 1 < k \leq k_0, \\ \xi_k \frac{\sigma_k}{\sigma_{k+1}} \sqrt{\frac{kk_0}{4\alpha^2-1} + \frac{k(k-k_0+1)}{2\alpha-1}} |L_{k_1}^{(k)}(0)| & \text{for } k_0 < k \leq n-1 \end{cases}$$



for moderately or mildly ill-posed problems with  $\sigma_j = \zeta j^{-\alpha}$ ,  $j = 1, 2, \dots, n$ , where  $\xi_k = \sqrt{\left(\frac{\|\Delta_k\|}{1+\|\Delta_k\|^2}\right)^2 + 1}$  for  $\|\Delta_k\| < 1$  and  $\xi_k \leq \frac{\sqrt{5}}{2}$  for  $\|\Delta_k\| \geq 1$  with  $\Delta_k$  defined by (3.11).

*Proof.* Since  $A_k$  is the best rank  $k$  approximation to  $A$  with respect to the 2-norm and  $\|A - A_k\| = \sigma_{k+1}$ , the lower bound in (4.2) holds. Next we prove the upper bound.

From (2.1), we obtain

$$(4.5) \quad \gamma_k = \|A - P_{k+1} B_k Q_k^T\| = \|A - A Q_k Q_k^T\| = \|A(I - Q_k Q_k^T)\|.$$

From Algorithm 1, (3.10), (3.12) and (3.13), we obtain

$$\mathcal{V}_k^R = \mathcal{K}_k(A^T A, A^T b) = \text{span}\{Q_k\} = \text{span}\{\hat{Z}_k\}$$

with  $Q_k$  and  $\hat{Z}_k$  being orthonormal, and the orthogonal projector onto  $\mathcal{V}_k^R$  is thus

$$(4.6) \quad Q_k Q_k^T = \hat{Z}_k \hat{Z}_k^T.$$

Keep in mind that  $A_k = U_k \Sigma_k V_k^T$ . It is direct to justify that  $(U_k \Sigma_k V_k^T)^T (A - U_k \Sigma_k V_k^T) = \mathbf{0}$  for  $k = 1, 2, \dots, n-1$ . Therefore, exploiting this and noting that  $\|I - \hat{Z}_k \hat{Z}_k^T\| = 1$  and  $V_k^T V_k^\perp = \mathbf{0}$  for  $k = 1, 2, \dots, n-1$ , we get from (4.5), (4.6) and (3.13) that

$$\begin{aligned} \gamma_k^2 &= \|(A - U_k \Sigma_k V_k^T + U_k \Sigma_k V_k^T)(I - \hat{Z}_k \hat{Z}_k^T)\|^2 \\ &= \max_{\|y\|=1} \|(A - U_k \Sigma_k V_k^T + U_k \Sigma_k V_k^T)(I - \hat{Z}_k \hat{Z}_k^T)y\|^2 \\ &= \max_{\|y\|=1} \|(A - U_k \Sigma_k V_k^T)(I - \hat{Z}_k \hat{Z}_k^T)y + U_k \Sigma_k V_k^T(I - \hat{Z}_k \hat{Z}_k^T)y\|^2 \\ &= \max_{\|y\|=1} \left( \|(A - U_k \Sigma_k V_k^T)(I - \hat{Z}_k \hat{Z}_k^T)y\|^2 + \|U_k \Sigma_k V_k^T(I - \hat{Z}_k \hat{Z}_k^T)y\|^2 \right) \\ &\leq \|(A - U_k \Sigma_k V_k^T)(I - \hat{Z}_k \hat{Z}_k^T)\|^2 + \|U_k \Sigma_k V_k^T(I - \hat{Z}_k \hat{Z}_k^T)\|^2 \\ &\leq \sigma_{k+1}^2 + \|\Sigma_k V_k^T(I - \hat{Z}_k \hat{Z}_k^T)\|^2 \\ &\leq \sigma_{k+1}^2 + \|\Sigma_k V_k^T (I - (V_k + V_k^\perp \Delta_k)(I + \Delta_k^T \Delta_k)^{-1}(V_k + V_k^\perp \Delta_k)^T) \|^2 \\ &= \sigma_{k+1}^2 + \|\Sigma_k (V_k^T - (I + \Delta_k^T \Delta_k)^{-1}(V_k + V_k^\perp \Delta_k)^T)\|^2 \\ &= \sigma_{k+1}^2 + \left\| \Sigma_k (I + \Delta_k^T \Delta_k)^{-1} \left( (I + \Delta_k^T \Delta_k) V_k^T - (V_k + V_k^\perp \Delta_k)^T \right) \right\|^2 \\ &= \sigma_{k+1}^2 + \|\Sigma_k (I + \Delta_k^T \Delta_k)^{-1} (\Delta_k^T \Delta_k V_k^T - \Delta_k^T (V_k^\perp)^T) \|^2 \\ (4.7) \quad &= \sigma_{k+1}^2 + \|\Sigma_k (I + \Delta_k^T \Delta_k)^{-1} \Delta_k^T \Delta_k V_k^T - \Sigma_k (I + \Delta_k^T \Delta_k)^{-1} \Delta_k^T (V_k^\perp)^T \|^2 \\ &\leq \sigma_{k+1}^2 + \|\Sigma_k (I + \Delta_k^T \Delta_k)^{-1} \Delta_k^T \Delta_k\|^2 + \|\Sigma_k (I + \Delta_k^T \Delta_k)^{-1} \Delta_k^T\|^2 \\ (4.8) \quad &= \sigma_{k+1}^2 + \epsilon_k^2, \end{aligned}$$

where the last inequality follows by using  $V_k^T V_k^\perp = \mathbf{0}$  and the definition of the induced matrix 2-norm to amplify the second term in (4.7).

We estimate  $\epsilon_k$  accurately below. To this end, we need to use two key identities and some results related. By the SVD of  $\Delta_k$ , it is direct to justify that

$$(4.9) \quad (I + \Delta_k^T \Delta_k)^{-1} \Delta_k^T \Delta_k = \Delta_k^T \Delta_k (I + \Delta_k^T \Delta_k)^{-1}$$

and

$$(4.10) \quad (I + \Delta_k^T \Delta_k)^{-1} \Delta_k^T = \Delta_k^T (I + \Delta_k \Delta_k^T)^{-1}.$$

Define the function  $f(\lambda) = \frac{\lambda}{1+\lambda^2}$  with  $\lambda \in [0, \infty)$ . Since the derivative  $f'(\lambda) = \frac{1-\lambda^2}{(1+\lambda^2)^2}$ ,  $f(\lambda)$  is monotonically increasing for  $\lambda \in [0, 1]$  and decreasing for  $\lambda \in [1, \infty)$ , and the maximum of  $f(\lambda)$  over  $\lambda \in [0, \infty)$  is  $\frac{1}{2}$ , which attains at  $\lambda = 1$ . Based on these properties and exploiting the SVD of  $\Delta_k$ , for the matrix 2-norm we get

$$(4.11) \quad \|\Delta_k (I + \Delta_k^T \Delta_k)^{-1}\| = \frac{\|\Delta_k\|}{1 + \|\Delta_k\|^2}$$

for  $\|\Delta_k\| < 1$  and

$$(4.12) \quad \|\Delta_k (I + \Delta_k^T \Delta_k)^{-1}\| \leq \frac{1}{2}$$

for  $\|\Delta_k\| \geq 1$  (Note: in this case, since  $\Delta_k$  may have at least one singular value smaller than one, we do not have an expression like (4.11)). It then follows from (4.8), (4.11), (4.12) and  $\|(1 + \Delta_k \Delta_k^T)^{-1}\| \leq 1$  that

$$(4.13) \quad \begin{aligned} \epsilon_k^2 &= \|\Sigma_k \Delta_k^T \Delta_k (I + \Delta_k^T \Delta_k)^{-1}\|^2 + \|\Sigma_k \Delta_k^T (I + \Delta_k \Delta_k^T)^{-1}\|^2 \\ &\leq \|\Sigma_k \Delta_k^T\|^2 \|\Delta_k (I + \Delta_k^T \Delta_k)^{-1}\|^2 + \|\Sigma_k \Delta_k^T\|^2 \|(1 + \Delta_k \Delta_k^T)^{-1}\|^2 \\ &\leq \|\Sigma_k \Delta_k^T\|^2 (\|\Delta_k (I + \Delta_k^T \Delta_k)^{-1}\|^2 + 1) \\ &= \|\Sigma_k \Delta_k^T\|^2 \left( \left( \frac{\|\Delta_k\|}{1 + \|\Delta_k\|^2} \right)^2 + 1 \right) = \xi_k^2 \|\Sigma_k \Delta_k^T\|^2 \end{aligned}$$

for  $\|\Delta_k\| < 1$  and

$$\epsilon_k \leq \|\Sigma_k \Delta_k^T\| \sqrt{\|\Delta_k (I + \Delta_k^T \Delta_k)^{-1}\|^2 + 1} = \xi_k \|\Sigma_k \Delta_k^T\| \leq \frac{\sqrt{5}}{2} \|\Sigma_k \Delta_k^T\|$$

for  $\|\Delta_k\| \geq 1$ . Replace  $\|\Sigma_k \Delta_k^T\|$  by its bounds (3.55) and (3.58) in the above, insert the resulting bounds for  $\epsilon_k$  into (4.8), and let  $\epsilon_k = \eta_k \sigma_{k+1}$ . Then we obtain the upper bound in (4.2) with  $\eta_k$  satisfying (4.3) and (4.4) for severely and moderately or mildly ill-posed problems, respectively.  $\square$

Note from (3.20) that

$$\frac{|u_{k+1}^T b|}{|u_k^T b|} = \frac{\sigma_{k+1}^{1+\beta}}{\sigma_k^{1+\beta}}, \quad k \leq k_0.$$

Therefore, for the right-hand side of (4.4) and  $k \leq k_0$  we have

$$\frac{\sigma_k}{\sigma_{k+1}} \frac{|u_{k+1}^T b|}{|u_k^T b|} = \left( \frac{\sigma_{k+1}}{\sigma_k} \right)^\beta < 1.$$

REMARK 4.1. For severely ill-posed problems, from (3.32), (3.33) and the definition of  $\xi_k$  we know that

$$\xi_k(1 + \mathcal{O}(\rho^{-2})) = 1 + \mathcal{O}(\rho^{-2})$$

for both  $k \leq k_0$  and  $k > k_0$ . Therefore, from (4.3) and (3.20), for  $k \leq k_0$  we have

$$(4.14) \quad \eta_k \leq \xi_k \frac{|u_{k+1}^T b|}{|u_k^T b|} (1 + \mathcal{O}(\rho^{-2})) = \frac{|u_{k+1}^T b|}{|u_k^T b|} = \frac{\sigma_{k+1}^{1+\beta}}{\sigma_k^{1+\beta}} = \mathcal{O}(\rho^{-1-\beta}) < 1$$

by ignoring the smaller term  $\mathcal{O}(\rho^{-1-\beta})\mathcal{O}(\rho^{-2}) = \mathcal{O}(\rho^{-3-\beta})$ , and for  $k > k_0$  we have

$$(4.15) \quad \eta_k \leq \xi_k \sqrt{k - k_0 + 1} (1 + \mathcal{O}(\rho^{-2})) = \sqrt{k - k_0 + 1}$$

by ignoring the smaller term  $\sqrt{k - k_0 + 1}\mathcal{O}(\rho^{-2})$ , which increases slowly with  $k$ .

REMARK 4.2. For the moderately or mildly ill-posed problems with  $\sigma_j = \zeta j^{-\alpha}$ , from the derivation on  $\eta_k$  and its estimate (4.4), by comparing (3.34) and (3.35) with (4.4), for  $k \leq k_0$  we approximately have

$$(4.16) \quad \frac{\sigma_k}{\sigma_{k+1}} \|\Delta_k\| \leq \eta_k \leq \frac{\sqrt{5}}{2} \frac{\sigma_k}{\sigma_{k+1}} \|\Delta_k\|,$$

and for  $k > k_0$ , from (3.42) and (3.43) we approximately have

$$(4.17) \quad \begin{aligned} \eta_k &< \frac{\sigma_k}{\sigma_{k+1}} \sqrt{\frac{kk_0}{4\alpha^2 - 1} + \frac{k(k - k_0 + 1)}{2\alpha - 1}} |L_{k_1}^{(k)}(0)| \\ &\sim \frac{k^{3/2}\sqrt{k_0}}{(2\alpha + 1)\sqrt{4\alpha^2 - 1}} + \frac{k^{3/2}\sqrt{k - k_0 + 1}}{(2\alpha + 1)\sqrt{2\alpha - 1}}, \end{aligned}$$

which increases faster than the right-hand side of (4.15) with respect to  $k$ .

REMARK 4.3. From (4.2), (4.3) and (4.14), for severely ill-posed problems we have

$$1 < \sqrt{1 + \eta_k^2} < 1 + \frac{1}{2}\eta_k^2 \leq 1 + \frac{1}{2} \frac{\sigma_{k+1}^{2(1+\beta)}}{\sigma_k^{2(1+\beta)}} \sim 1 + \frac{1}{2}\rho^{-2(1+\beta)},$$

and  $\gamma_k$  is an accurate approximation to  $\sigma_{k+1}$  for  $k \leq k_0$  and marginally less accurate for  $k > k_0$ . Thus, the rank  $k$  approximation  $P_{k+1}B_kQ_k^T$  is as accurate as the best rank  $k$  approximation  $A_k$  within the factor  $\sqrt{1 + \eta_k^2} \approx 1$  for  $k \leq k_0$  and  $\rho > 1$  suitably. For moderately ill-posed problems,  $\gamma_k$  is still an excellent approximation to  $\sigma_{k+1}$ , and the rank  $k$  approximation  $P_{k+1}B_kQ_k^T$  is almost as accurate as the best rank  $k$  approximation  $A_k$  for  $k \leq k_0$ . Therefore,  $P_{k+1}B_kQ_k^T$  plays the same role as  $A_k$  for these two kinds of ill-posed problems and  $k \leq k_0$ , it is known from the clarification in Section 2 that LSQR may have the full regularization. We will, afterwards, deepen this theorem and derive more results, proving that LSQR must have the full regularization for these two kinds of problems provided that  $\rho > 1$  and  $\alpha > 1$  suitably.

For both severely and moderately ill-posed problems, we note that the situation is not so satisfying for increasing  $k > k_0$ . But at that time, a possibly big  $\eta_k$  does not do harm to our regularization purpose since we will prove that, provided that  $\rho > 1$  and  $\alpha > 1$  suitably, LSQR has the full regularization and has already found a best possible regularized solution at semi-convergence occurring at iteration  $k_0$ . If it is the case, we will simply stop performing it after semi-convergence.

REMARK 4.4. For mildly ill-posed problems, the situation is fundamentally different. As clarified in Remark 3.8, we have  $\sqrt{\frac{k^2}{4\alpha^2 - 1} + \frac{k}{2\alpha - 1}} > 1$  and  $|L_k^{(k)}(0)| > 1$

considerably as  $k$  increases up to  $k_0$  because of  $\frac{1}{2} < \alpha \leq 1$ , leading to  $\eta_k > 1$  substantially. This means that  $\gamma_{k_0}$  is substantially bigger than  $\sigma_{k_0+1}$  and can well lie between  $\sigma_{k_0}$  and  $\sigma_1$ , so that the rank  $k_0$  approximation  $P_{k_0+1}B_{k_0}Q_{k_0}^T$  is much less accurate than the best rank  $k_0$  approximation  $A_{k_0}$  and LSQR has only the partial regularization.

REMARK 4.5. For a given ill-posed problem, the noise level  $\|e\|$  only affects  $k_0$  but has no effect on the overall decay rate of  $\gamma_k$ .

REMARK 4.6. There are several subtle treatments in the proof of Theorem 4.1, each of which turns out to be absolutely necessary. Ignoring or missing any one of them would be fatal and make us fail to obtain accurate estimates for  $\epsilon_k$  defined by (4.8): The first is the treatment of  $\|U_k \Sigma_k V_k^T (I - \hat{Z}_k \hat{Z}_k^T)\|$ . By the definition of  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$ , if we had amplified it by

$$\|U_k \Sigma_k V_k^T (I - \hat{Z}_k \hat{Z}_k^T)\| \leq \|\Sigma_k\| \|V_k^T (I - \hat{Z}_k \hat{Z}_k^T)\| = \sigma_1 \|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|,$$

we would have obtained a too large overestimate, which is almost a fixed constant for severely ill-posed problems and  $k = 1, 2, \dots, k_0$  and increases with  $k = 1, 2, \dots, k_0$  for moderately and mildly ill-posed problems. Such rough estimates are useless to get a meaningful bound for  $\gamma_k$ . The key is to treat  $U_k \Sigma_k V_k^T (I - \hat{Z}_k \hat{Z}_k^T)$  as a whole other rather separate it in the above way, so that we can bound its norm accurately. The second is the use of (4.9) and (4.10). The third is the extraction of  $\|\Sigma_k \Delta_k^T\|$  from (4.13) as a whole other than amplify it to  $\|\Sigma_k\| \|\Delta_k\| = \sigma_1 \|\Delta_k\|$ , i.e., the fatal overestimate (3.62). The fourth is accurate estimates for it; see (3.55) and (3.58) in Theorem 3.5. For example, without using (4.9) and (4.10), we would have no way but to obtain

$$\begin{aligned} \epsilon_k^2 &\leq \|\Sigma_k\|^2 \|(I + \Delta_k^T \Delta_k)^{-1} \Delta_k^T \Delta_k\|^2 + \|\Sigma_k\|^2 \|(I + \Delta_k^T \Delta_k)^{-1} \Delta_k^T\|^2 \\ &= \sigma_1^2 \left( \frac{\|\Delta_k\|^2}{1 + \|\Delta_k\|^2} \right)^2 + \sigma_1^2 \|(I + \Delta_k^T \Delta_k)^{-1} \Delta_k^T\|^2 \\ &= \sigma_1^2 \left( \frac{\|\Delta_k\|^2}{1 + \|\Delta_k\|^2} \right)^2 + \sigma_1^2 \|\Delta_k (I + \Delta_k^T \Delta_k)^{-1}\|^2. \end{aligned}$$

From (4.11), (4.12) and the previous estimates for  $\|\Delta_k\|$ , such bound is too pessimistic and completely useless in our context, and it even does not decrease and could not be small as  $k$  increases, while our estimates for  $\epsilon_k = \eta_k \sigma_{k+1}$  in Theorem 4.1 are much more accurate and decay swiftly as  $k$  increases, as indicated by (4.3) and (4.4).

In order to prove the full or partial regularization of LSQR for (1.1) completely and rigorously, besides Theorem 4.1, it appears that we need to introduce a precise definition of the near best rank  $k$  approximation  $P_{k+1}B_kQ_k^T$  to  $A$ , i.e., the precise meaning of  $\gamma_k \approx \sigma_{k+1}$ . By definition (4.1), the rank  $k$  matrix  $P_{k+1}B_kQ_k^T$  is called a near best rank  $k$  approximation to  $A$  if it satisfies

$$(4.18) \quad \sigma_{k+1} \leq \gamma_k < \sigma_k \text{ and } \gamma_k - \sigma_{k+1} < \sigma_k - \gamma_k, \text{ i.e., } \gamma_k < \frac{\sigma_k + \sigma_{k+1}}{2},$$

that is,  $\gamma_k$  lies between  $\sigma_k$  and  $\sigma_{k+1}$  and is closer to  $\sigma_{k+1}$ . This definition is natural. For an ill-posed problem (1.1), since there is no considerable gap of  $\sigma_k$  and  $\sigma_{k+1}$ , the definition means that  $\gamma_k$  must approximate  $\sigma_{k+1}$  more accurately as  $k$  increases. We mention in passing that a near best rank  $k$  approximation to  $A$  from an ill-posed problem is much more stringent than it is for a matrix from a (numerically) rank-deficient problem where the large singular values are very well separated from

the small ones and there is a substantial gap between two groups of singular values. In addition, we point out that it may be much harder to computationally obtain a near best  $k$  rank approximation to the large  $A$  from the ill-posed problem than for a numerically rank deficient matrix of the same order.

Based on Theorem 4.1, for the severely and moderately or mildly ill-posed problems with the singular value models  $\sigma_k = \zeta\rho^{-k}$  and  $\sigma_k = \zeta k^{-\alpha}$ , we next derive the sufficient conditions on  $\rho$  and  $\alpha$  that guarantee that  $P_{k+1}B_kQ_k^T$  is a near best rank  $k$  approximation to  $A$  for  $k = 1, 2, \dots, k_0$ . We analyze if and how the sufficient conditions are satisfied for three kinds of ill-posed problems.

**THEOREM 4.2.** *For a given (1.1), assume that the discrete Picard condition (1.6) is satisfied. Then, in the sense of (4.18),  $P_{k+1}B_kQ_k^T$  is a near best rank  $k$  approximation to  $A$  for  $k = 1, 2, \dots, k_0$  if*

$$(4.19) \quad \sqrt{1 + \eta_k^2} < \frac{1}{2} \frac{\sigma_k}{\sigma_{k+1}} + \frac{1}{2}.$$

*For the severely ill-posed problems with  $\sigma_k = \zeta\rho^{-k}$  and the moderately or mildly ill-posed problems with  $\sigma_k = \zeta k^{-\alpha}$ ,  $P_{k+1}B_kQ_k^T$  is a near best rank  $k$  approximation to  $A$  for  $k = 1, 2, \dots, k_0$  if  $\rho > 2$  and  $\alpha$  satisfies*

$$(4.20) \quad 2\sqrt{1 + \eta_k^2} - 1 < \left( \frac{k_0 + 1}{k_0} \right)^\alpha,$$

*respectively.*

*Proof.* By (4.2), we see that  $\gamma_k \leq \sqrt{1 + \eta_k^2} \sigma_{k+1}$ . Therefore,  $P_{k+1}B_kQ_k^T$  is a near best rank  $k$  approximation to  $A$  in the sense of (4.18) provided that

$$\sqrt{1 + \eta_k^2} \sigma_{k+1} < \sigma_k$$

and

$$\sqrt{1 + \eta_k^2} \sigma_{k+1} < \frac{\sigma_k + \sigma_{k+1}}{2},$$

from which (4.19) follows.

From (4.14), for the severely ill-posed problems with  $\sigma_k = \zeta\rho^{-k}$  and  $\rho > 1$  we have

$$(4.21) \quad \sqrt{1 + \eta_k^2} < 1 + \frac{1}{2} \eta_k^2 \leq 1 + \frac{1}{2} \rho^{-2(1+\beta)} < 1 + \rho^{-1}, \quad k = 1, 2, \dots, k_0,$$

from which it follows that

$$(4.22) \quad \sqrt{1 + \eta_k^2} \sigma_{k+1} < (1 + \rho^{-1}) \sigma_{k+1}.$$

Since  $\sigma_k/\sigma_{k+1} = \rho$ , (4.19) holds provided that

$$1 + \rho^{-1} < \frac{1}{2} \rho + \frac{1}{2},$$

i.e.,  $\rho^2 - \rho - 2 > 0$ , solving which for  $\rho$  we get  $\rho > 2$ . For the moderately or mildly ill-posed problems with  $\sigma_k = \zeta k^{-\alpha}$ , it is direct from (4.19) to get

$$2\sqrt{1 + \eta_k^2} - 1 < \left( \frac{k+1}{k} \right)^\alpha.$$

Since  $\left(\frac{k+1}{k}\right)^\alpha$  decreases monotonically as  $k$  increases, its minimum over  $k = 1, 2, \dots, k_0$  is  $\left(\frac{k_0+1}{k_0}\right)^\alpha$ . Therefore, we obtain (4.20).  $\square$

REMARK 4.7. Given the noise level  $\|e\|$ , the discrete Picard condition (1.6) and (1.7), from the bound (4.4) for  $\eta_k$ ,  $k = 1, 2, \dots, k_0$ , we see that the bigger  $\alpha > 1$  is, the smaller  $k_0$  and  $\eta_k$  are. Therefore, there must be  $\alpha > 1$  such that (4.20) holds. Here we should remind that it is more suitable to regard the conditions on  $\rho$  and  $\alpha$  as an indication that  $\rho$  and  $\alpha$  must not be close to one other than precise requirements since we have used the bigger (4.21) and simplified models  $\sigma_k = \zeta\rho^{-k}$  and  $\sigma_k = \zeta k^{-\alpha}$ .

REMARK 4.8. For the mildly ill-posed problems with  $\sigma_k = \zeta k^{-\alpha}$ , Theorem 3.3 has shown that  $\|\Delta_k\|$  is generally not small and can be arbitrarily large for  $k = 1, 2, \dots, k_0$ . From (4.16), we see that  $\eta_k$  has comparable size to  $\|\Delta_k\|$ . Note that the right-hand side  $\left(\frac{k_0+1}{k_0}\right)^\alpha \leq 2$  for  $\frac{1}{2} < \alpha \leq 1$  and any  $k_0 \geq 1$ . Consequently, (4.20) cannot be met generally for mildly ill-posed problems. The rare possible exceptions are that  $k_0$  is only very few and  $\alpha$  is close to one since, in such case,  $\eta_k$  is not large for  $k = 1, 2, \dots, k_0$ . So,  $P_{k+1}B_kQ_k^T$  is generally not a near best rank  $k$  approximation to  $A$  for  $k = 1, 2, \dots, k_0$  for this kind of problem.

**4.2. The approximation behavior of the Ritz values  $\theta_i^{(k)}$ .** In this subsection, starting with Theorem 4.1, we prove that, under certain sufficient conditions on  $\rho$  and  $\alpha$  for the severely and moderately ill-posed problems with the models  $\sigma_i = \zeta\rho^{-i}$  and  $\sigma_i = \zeta i^{-\alpha}$ , respectively, the  $k$  Ritz values  $\theta_i^{(k)}$  approximate the first  $k$  large singular values  $\sigma_i$  in natural order for  $k = 1, 2, \dots, k_0$ , which means that no Ritz value smaller than  $\sigma_{k_0+1}$  appears. Combining this result with Theorem 4.2, we can draw the definite conclusion that LSQR must have the full regularization for these two kinds of problems provided that  $\rho > 1$  and  $\alpha > 1$  suitably.

THEOREM 4.3. Assume that (1.1) is severely ill-posed with  $\sigma_i = \zeta\rho^{-i}$  and  $\rho > 1$  or moderately ill-posed with  $\sigma_i = \zeta i^{-\alpha}$  and  $\alpha > 1$ , and the discrete Picard condition (1.6) is satisfied. Let the Ritz values  $\theta_i^{(k)}$  be labeled as  $\theta_1^{(k)} > \theta_2^{(k)} > \dots > \theta_k^{(k)}$ . Then

$$(4.23) \quad 0 < \sigma_i - \theta_i^{(k)} \leq \sqrt{1 + \eta_k^2 \sigma_{k+1}}, \quad i = 1, 2, \dots, k.$$

If  $\rho \geq 1 + \sqrt{2}$  or  $\alpha > 1$  satisfies

$$(4.24) \quad 1 + \sqrt{1 + \eta_k^2} < \left(\frac{k_0 + 1}{k_0}\right)^\alpha, \quad k = 1, 2, \dots, k_0,$$

then the  $k$  Ritz values  $\theta_i^{(k)}$  strictly interlace the first large  $k + 1$  singular values of  $A$  and approximate the first  $k$  large ones in natural order for  $k = 1, 2, \dots, k_0$ :

$$(4.25) \quad \sigma_{i+1} < \theta_i^{(k)} < \sigma_i, \quad i = 1, 2, \dots, k,$$

meaning that there is no Ritz value  $\theta_i^{(k)}$  smaller than  $\sigma_{k_0+1}$  for  $k = 1, 2, \dots, k_0$ .

*Proof.* Note that for  $k = 1, 2, \dots, k_0$  the  $\theta_i^{(k)}$ ,  $i = 1, 2, \dots, k$  are just the nonzero singular values of  $P_{k+1}B_kQ_k^T$ , whose other  $n - k$  singular values are zeros. We write

$$A = P_{k+1}B_kQ_k^T + (A - P_{k+1}B_kQ_k^T)$$

with  $\|A - P_{k+1}B_kQ_k^T\| = \gamma_k$  by definition (4.1). Then by the Mirsky's theorem of singular values [109, p.204, Thm 4.11], we have

$$(4.26) \quad |\sigma_i - \theta_i^{(k)}| \leq \gamma_k \leq \sqrt{1 + \eta_k^2 \sigma_{k+1}}, \quad i = 1, 2, \dots, k.$$



Since the singular values of  $A$  are simple and  $b$  has components in all the left singular vectors  $u_1, u_2, \dots, u_n$  of  $A$ , Lanczos bidiagonalization, i.e., Algorithm 1, can be run to completion, producing  $P_{n+1}$ ,  $Q_n$  and the lower bidiagonal  $B_n \in \mathbb{R}^{(n+1) \times n}$  such that

$$(4.27) \quad P^T A Q_n = \begin{pmatrix} B_n \\ \mathbf{0} \end{pmatrix}$$

with the  $m \times m$  matrix  $P = (P_{n+1}, \hat{P})$  and  $n \times n$  matrix  $Q_n$  orthogonal and all the  $\alpha_i$  and  $\beta_{i+1}$ ,  $i = 1, 2, \dots, n$ , of  $B_n$  being positive. Note that the singular values of  $B_k$ ,  $k = 1, 2, \dots, n$ , are all simple and that  $B_k$  consists of the first  $k$  columns of  $B_n$  with the last  $n-k$  zero rows deleted. Applying the Cauchy's *strict* interlacing theorem [109, p.198, Corollary 4.4] to the singular values of  $B_k$  and  $B_n$ , we have

$$(4.28) \quad \sigma_{n-k+i} < \theta_i^{(k)} < \sigma_i, \quad i = 1, 2, \dots, k.$$

Therefore, (4.26) becomes

$$(4.29) \quad 0 < \sigma_i - \theta_i^{(k)} \leq \gamma_k \leq \sqrt{1 + \eta_k^2} \sigma_{k+1}, \quad i = 1, 2, \dots, k,$$

which proves (4.23). That is, the  $\theta_i^{(k)}$  approximate  $\sigma_i$  from below for  $i = 1, 2, \dots, k$  with the errors no more than  $\gamma_k \leq \sqrt{1 + \eta_k^2} \sigma_{k+1}$ . For  $i = 1, 2, \dots, k$ , notice that  $\rho^{-k+i} \leq 1$ . Then from (4.29), (4.21) and  $\sigma_i = \zeta \rho^{-i}$  we obtain

$$\begin{aligned} \theta_i^{(k)} &\geq \sigma_i - \gamma_k > \sigma_i - (1 + \rho^{-1}) \sigma_{k+1} \\ &= \zeta \rho^{-i} - \zeta (1 + \rho^{-1}) \rho^{-(k+1)} \\ &= \zeta \rho^{-(i+1)} (\rho - (1 + \rho^{-1}) \rho^{-k+i}) \\ &\geq \zeta \rho^{-(i+1)} (\rho - \rho^{-1} - 1) \\ &\geq \zeta \rho^{-(i+1)} = \sigma_{i+1}, \end{aligned}$$

provided that  $\rho - \rho^{-1} \geq 2$ , solving which we get  $\rho \geq 1 + \sqrt{2}$ . Together with the upper bound of (4.28), we have proved (4.25).

For the moderately ill-posed problems with  $\sigma_i = \zeta i^{-\alpha}$ ,  $i = 1, 2, \dots, k$  and  $k = 1, 2, \dots, k_0$ , we get

$$\begin{aligned} \theta_i^{(k)} &\geq \sigma_i - \gamma_k \geq \sigma_i - \sqrt{1 + \eta_k^2} \sigma_{k+1} \\ &= \zeta i^{-\alpha} - \zeta \sqrt{1 + \eta_k^2} (k+1)^{-\alpha} \\ &= \zeta (i+1)^{-\alpha} \left( \left( \frac{i+1}{i} \right)^\alpha - \sqrt{1 + \eta_k^2} \left( \frac{i+1}{k+1} \right)^\alpha \right) \\ &> \zeta (i+1)^{-\alpha} = \sigma_{i+1}, \end{aligned}$$

i.e., (4.25) holds, provided that  $\eta_k > 0$  and  $\alpha > 1$  are such that

$$\left( \frac{i+1}{i} \right)^\alpha - \sqrt{1 + \eta_k^2} \left( \frac{i+1}{k+1} \right)^\alpha > 1,$$

which means that

$$\sqrt{1 + \eta_k^2} < \left( \left( \frac{i+1}{i} \right)^\alpha - 1 \right) \left( \frac{k+1}{i+1} \right)^\alpha = \left( \frac{k+1}{i} \right)^\alpha - \left( \frac{k+1}{i+1} \right)^\alpha, \quad i = 1, 2, \dots, k.$$

It is easily justified that the above right-hand side monotonically decreases with respect to  $i = 1, 2, \dots, k$ , whose minimum attains at  $i = k$  and equals  $(\frac{k+1}{k})^\alpha - 1$ . Furthermore, since  $(\frac{k+1}{k})^\alpha - 1$  decreases monotonically as  $k$  increases, its minimum over  $k = 1, 2, \dots, k_0$  is  $(\frac{k_0+1}{k_0})^\alpha - 1$ , which is just the condition (4.24).  $\square$

REMARK 4.9. *Similar to (4.20), there must be  $\alpha > 1$  such that (4.24) holds. Again, we stress that the conditions on  $\rho$  and  $\alpha$  should be regarded as an indicator that  $\rho$  and  $\alpha$  must not be close to one other than precise requirements since we have used the amplified (4.21) and the simplified models  $\sigma_i = \zeta\rho^{-i}$  and  $\sigma_i = \zeta i^{-\alpha}$ . Comparing Theorem 4.2 with Theorem 4.3, we find out that, as far as the severely or moderately ill-posed problems are concerned, for  $k = 1, 2, \dots, k_0$  the near best rank approximation  $P_{k+1}B_kQ_k^T$  essentially means that the singular values  $\theta_i^{(k)}$  of  $B_k$  approximate the first  $k$  large singular values  $\sigma_i$  of  $A$  in natural order, provided that  $\rho > 1$  or  $\alpha > 1$  suitably.*

REMARK 4.10. *Under the conditions of Theorems 4.2–4.3, let us explore how the results in them depend on  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$ . (4.14) and (3.8) indicate that, for the severely ill-posed problems with  $\sigma_k = \zeta\rho^{-k}$ , ignoring higher order small terms, we have  $\eta_k \leq \rho^{-1-\beta}$  and  $\|\Delta_k\| \leq \rho^{-2-\beta} < 1$  for  $k \leq k_0$ ; for the moderately ill-posed problems with  $\sigma_k = \zeta k^{-\alpha}$ , (4.16) indicates that  $\eta_k$  and  $\|\Delta_k\|$  are comparable in size for  $k \leq k_0$ , while (3.37) shows that  $\|\Delta_k\|$  is at most of modest size for  $k \leq k_0$ . As a result, Theorem 3.1 and Theorem 3.3 demonstrate that  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\| < \frac{1}{\sqrt{2}}$  and  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\| < 1$  fairly for severely and moderately ill-posed problems, respectively. In other words, the largest canonical angle between  $\mathcal{V}_k^R$  and  $\mathcal{V}_k$  does not exceed  $\frac{\pi}{4}$  and is considerably smaller than  $\frac{\pi}{2}$  for these two kinds of problems and  $k \leq k_0$ , respectively.*

REMARK 4.11. *Theorems 4.1–4.3 show that, for  $k = 1, 2, \dots, k_0$ , the  $k$ -step Lanczos bidiagonalization is guaranteed to extract or acquire the first  $k$  dominant SVD components for the severely or moderately ill-posed problems with  $\rho > 1$  or  $\alpha > 1$  suitably, so that LSQR has the full regularization for these two kinds of ill-posed problems and can obtain best possible regularized solutions  $x^{(k_0)}$  at semi-convergence.*

Let us have a closer look at the regularization of LSQR for mildly ill-posed problems. We observe that the sufficient condition (4.24) for (4.25) is never met for this kind of problem because  $(\frac{k_0+1}{k_0})^\alpha \leq 2$  for any  $k_0$  and  $\frac{1}{2} < \alpha \leq 1$ . This indicates that, for  $k = 1, 2, \dots, k_0$ , the  $k$  Ritz values  $\theta_i^{(k)}$  may not approximate the first  $k$  large singular values  $\sigma_i$  in natural order and particularly there is at least one Ritz value  $\theta_{k_0}^{(k_0)} < \sigma_{k_0+1}$ , causing that  $x^{(k_0)}$  is already deteriorated and cannot be as accurate as the best TSVD solution  $x_{k_0}^{tsvd}$ , so that LSQR has only the partial regularization. We can also make use of Theorem 3.4 to explain the partial regularization of LSQR: Theorem 3.3 has shown that  $\|\Delta_k\|$  is generally not small and may become arbitrarily large as  $k$  increases up to  $k_0$  for mildly ill-posed problems, meaning that  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\| \approx 1$ , as the sharp bound (3.37) indicates, from which it follows that a small Ritz value  $\theta_{k_0}^{(k_0)} < \sigma_{k_0+1}$  generally appears.

**4.3. General best or best rank  $k$  approximations to  $A$  and their implications on LSQR.** We investigate the general best or near best rank  $k$  approximations to  $A$  with  $\sigma_k = \zeta k^{-\alpha}$  and  $\alpha > \frac{1}{2}$ . We aim to show that, for each of such rank  $k$  approximations, its smallest nonzero singular value may be smaller than  $\sigma_{k+1}$  for  $\frac{1}{2} < \alpha \leq 1$ , that is, its nonzero singular values may not approximate the  $k$  large singular values of  $A$  in natural order, while the smallest nonzero singular value of such a rank  $k$  approximation is guaranteed to be bigger than  $\sigma_{k+1}$  if only  $\alpha > 1$  suitably. As it will turn out, this can help us further understand the regularization of LSQR for mildly

and moderately ill-posed problems. Finally, we investigate the behavior of the Ritz values  $\theta_i^{(k)}$ ,  $i = 1, 2, \dots, k$  when  $P_{k+1}B_kQ_k^T$  is not a near best rank  $k$  approximation to  $A$  for mildly ill-posed problems.

First of all, we point out an intrinsic fact that both the best and near best rank  $k$  approximations to  $A$  with respect to the 2-norm are *not* unique. This fact is important for further understanding Theorem 4.3.

Let  $C_k$  be a best or near best rank  $k$  approximation to  $A$  with  $\|A - C_k\| = (1 + \epsilon)\sigma_{k+1}$  with any  $\epsilon \geq 0$  satisfying  $(1 + \epsilon)\sigma_{k+1} < \frac{\sigma_k + \sigma_{k+1}}{2}$  (Note:  $\epsilon = 0$  corresponds to a best rank  $k$  approximation), i.e.,  $(1 + \epsilon)\sigma_{k+1}$  is between  $\sigma_{k+1}$  and  $\sigma_k$  and closer to  $\sigma_{k+1}$ , by which we get

$$1 + 2\epsilon < \frac{\sigma_k}{\sigma_{k+1}}.$$

It is remarkable to note that  $C_k$  is not unique. For example, among others, all the

$$C_k = A_k(\theta, j) = A_k - \sigma_{k+1} U_k \text{diag}(\theta(1+\epsilon), \dots, \theta(1+\epsilon), \underbrace{(1+\epsilon), \theta(1+\epsilon), \dots, \theta(1+\epsilon)}_j) V_k^T$$

with any  $0 \leq \theta \leq 1$  and  $1 \leq j \leq k-1$  is a family of best or near best rank  $k$  approximations to  $A$ . The smallest nonzero singular value of  $A_k(\theta, j)$  is  $\sigma_k - \theta(1 + \epsilon)\sigma_{k+1}$ . Since  $\sigma_k = \zeta k^{-\alpha}$  and  $\left(\frac{k+1}{k}\right)^\alpha < 2$  for any  $k > 1$  and  $\frac{1}{2} < \alpha \leq 1$ , we obtain

$$(4.30) \quad \sigma_k - \theta(1 + \epsilon)\sigma_{k+1} = \sigma_{k+1} \left( \left( \frac{k+1}{k} \right)^\alpha - \theta(1 + \epsilon) \right) < \sigma_{k+1}$$

for  $\theta$  sufficiently close to one. This shows that  $\sigma_k - \theta(1 + \epsilon)\sigma_{k+1}$  does not lie between  $\sigma_{k+1}$  and  $\sigma_k$  and interlace them for  $k > 1$ . In this case, for a given  $\alpha \in (\frac{1}{2}, 1]$ , the bigger  $k$  is, the smaller  $\left(\frac{k+1}{k}\right)^\alpha - \theta(1 + \epsilon)$  is, and the further is  $\sigma_k - \theta(1 + \epsilon)\sigma_{k+1}$  away from  $\sigma_{k+1}$ . On the other hand, for  $\theta$  sufficiently small we have

$$(4.31) \quad \left( \frac{k+1}{k} \right)^\alpha - \theta(1 + \epsilon) > 1,$$

that is,  $\sigma_k - \theta(1 + \epsilon)\sigma_{k+1}$  interlaces  $\sigma_{k+1}$  and  $\sigma_k$  for  $\theta$  sufficiently small.

For  $A$  with  $\sigma_k = \zeta k^{-\alpha}$  and  $\alpha > 1$ , the situation is much better since, for any  $k$ , the requirement (4.31) is met for *any*  $0 \leq \theta \leq 1$  provided that  $\alpha > 1$  suitably, leading to  $\sigma_k - \theta(1 + \epsilon)\sigma_{k+1} > \sigma_{k+1}$ , meaning that the smallest singular value  $\sigma_k - \theta(1 + \epsilon)\sigma_{k+1}$  of a near best rank approximation  $A_k(\theta, j)$  interlaces  $\sigma_{k+1}$  and  $\sigma_k$ .

However, we should be aware that the above analysis is made for the *worst-case*: For any best or a near best rank  $k$  approximation  $C_k$  to  $A$ , the minimum of the smallest nonzero singular values of all the  $C_k$  is exactly  $\sigma_k - (1 + \epsilon)\sigma_{k+1}$ . We now prove this. Suppose that  $\sigma_k(C_k)$  is the smallest nonzero singular value of a given such  $C_k$ . Then from  $\|A - C_k\| = (1 + \epsilon)\sigma_{k+1}$ , by the standard perturbation theory we have

$$|\sigma_k - \sigma_k(C_k)| \leq (1 + \epsilon)\sigma_{k+1}.$$

Clearly, the minimum of all the  $\sigma_k(C_k)$  is attained if and only if the above equality holds, which is exactly  $\sigma_k - (1 + \epsilon)\sigma_{k+1}$ . On the other side, by construction, we also see that the smallest singular value  $\sigma_k - \theta(1 + \epsilon)\sigma_{k+1}$  of  $C_k$  is arbitrarily close to or equal to  $\sigma_k$  by taking  $\theta$  arbitrarily small or zero, which means that (4.31) holds. In

this case, we observe from the equality in (4.30) that  $\sigma_k - \theta(1 + \epsilon)\sigma_{k+1} > \sigma_{k+1}$  and interlaces  $\sigma_{k+1}$  and  $\sigma_k$ .

As far as LSQR is concerned, notice that the condition (4.24) for the interlacing property (4.25) is derived by assuming the worst case that  $\sigma_k - \theta_k^{(k)} = \gamma_k \leq \sqrt{1 + \eta_k^2}\sigma_{k+1}$ , i.e.,  $\theta_k^{(k)}$  is supposed to be the smallest possible nonzero one among all the  $\sigma_k(C_k)$ , where  $C_k$  belongs to the set of near best  $k$  approximations that satisfy  $\|A - C_k\| = \gamma_k \leq \sqrt{1 + \eta_k^2}\sigma_{k+1}$ . For mildly ill-posed problems, the above arguments indicate that although in the worst case some of the  $k$  Ritz values  $\theta_i^{(k)}$  may not approximate the first  $k$  large singular values  $\sigma_i$  of  $A$  in natural order, it is possible so in practice in case  $P_{k+1}B_kQ_k^T$  is *occasionally* a near best rank  $k$  approximation to  $A$  for some small  $k \leq k_0$ .

Unfortunately, as we have shown previously,  $P_{k+1}B_kQ_k^T$  is rarely a near best rank  $k$  approximation to  $A$  for mildly ill-posed problems, i.e.,  $\gamma_k > \sigma_k$  generally. Recall the second part of Theorem 3.4 and Remark 3.12, which have shown rigorously that there is at least one Ritz value  $\theta_k^{(k)} < \sigma_{k+1}$  if  $\varepsilon_k$  is sufficiently small there, that is,  $\eta_k$  or equivalently  $\|\Delta_k\|$  is large. This is exactly the case that  $P_{k+1}B_kQ_k^T$  is not a near best rank  $k$  approximation to  $A$ , causing that LSQR has only the partial regularization.

We can make a further analysis on the behavior of  $\theta_i^{(k)}$ ,  $i = 1, 2, \dots, k$  when (1.1) is mildly ill-posed. Suppose that  $\gamma_k \in [\sigma_{j+1}, \sigma_j]$  for some  $j \leq k$ , which means that  $P_{k+1}B_kQ_k^T$  is definitely not a near best rank  $k$  approximation to  $A$  when  $j < k$ . Below we derive the smallest upper bound for  $\sigma_j - \gamma_k$  and obtain the biggest lower bound for  $\theta_j^{(k)}$ . For  $\sigma_j = \zeta j^{-\alpha}$  with  $\frac{1}{2} < \alpha \leq 1$  we have

$$\begin{aligned} \sigma_j - \gamma_k &\leq \sigma_j - \sigma_{j+1} = \sigma_{j+1} \left( \left( \frac{j+1}{j} \right)^\alpha - 1 \right) \\ &\leq \sigma_{j+1} \left( 1 + \frac{\alpha}{j} - 1 \right) \\ &= \frac{\alpha}{j} \sigma_{j+1} = \frac{\alpha}{\zeta j^{1-\alpha}} \zeta j^{-\alpha} \sigma_{j+1} = \frac{\alpha}{\zeta j^{1-\alpha}} \zeta^2 j^{-\alpha} (j+1)^{-\alpha} \\ &= \frac{\alpha}{\zeta j^{1-\alpha}} \zeta \sigma_{j(j+1)} = \frac{\alpha}{j^{1-\alpha}} \sigma_{j(j+1)}, \end{aligned}$$

in which  $\frac{\alpha}{j^{1-\alpha}} < 1$  decreases with increasing  $j$  for  $\alpha < 1$  and is one for  $\alpha = 1$ . Therefore, the smallest upper bound for  $\sigma_j - \gamma_k$  is no more than  $\sigma_{j(j+1)}$ , which is smaller than  $\sigma_{k+1}$  once  $j(j+1) > k$ . In view of the above and (4.29), for  $\gamma_k \in [\sigma_{j+1}, \sigma_j]$ , since  $\theta_j^{(k)} \geq \sigma_j - \gamma_k$  and has the biggest lower bound  $\sigma_{j(j+1)}$ , we may have  $\theta_j^{(k)} < \sigma_{k+1}$  provided that  $j(j+1) > k$ . Moreover, when  $\theta_j^{(k)} < \sigma_{k+1}$ , by the labeling rule, there are  $k - j + 1$  Ritz values  $\theta_j^{(k)}, \theta_{j+1}^{(k)}, \dots, \theta_k^{(k)}$  smaller than  $\sigma_{k+1}$ . As a result, for  $k = k_0$ , there are  $k_0 - j + 1$  Ritz values smaller than  $\sigma_{k_0+1}$  that deteriorate the LSQR iterate  $x^{(k_0)}$ , so that LSQR has only the partial regularization.

**5. Decay rates of  $\alpha_k$  and  $\beta_{k+1}$  and the regularization of LSMR and CGME.** In this section, we will present a number of results on the decay rates of  $\alpha_k$ ,  $\beta_{k+1}$  and  $\gamma_k$  and on certain other rank  $k$  approximations to  $A$  and  $A^T A$  constructed by Lanczos bidiagonalization. The decay rates of  $\alpha_k$  and  $\beta_{k+1}$  are particularly useful for practically detecting the degree of ill-posedness of (1.1) and identifying the full or partial regularization of LSQR and LSMR. The results on the new rank  $k$  approximations critically determine the full or partial regularization of the Krylov iterative regularization solvers LSMR [30] and CGME [22, 45, 47, 61]. In Section 5.1,

we prove how  $\alpha_k$  and  $\beta_{k+1}$  decay by relating them to  $\gamma_k$  and the estimates established for it. Then we show how to exploit the decay rate of  $\alpha_k + \beta_{k+1}$  to identify the degree of ill-posedness of (1.1) and the regularization of LSQR. In Section 5.2, we prove that the regularization of LSMR resembles LSQR for each of the three kinds of ill-posed problems. In Section 5.3, we prove that the regularizing effects of CGME have intrinsic indeterminacy and are inferior to those of LSQR and LSMR. In Section 5.4, we compare LSQR with some standard randomized algorithms [43] and strong rank-revealing QR, i.e., RRQR, factorizations [42, 63], and show that the former solves ill-posed problems more accurately than the latter two ones at no more cost.

**5.1. Decay rates of  $\alpha_k$  and  $\beta_{k+1}$  and their practical use.** We consider how  $\alpha_k$  and  $\beta_{k+1}$  decay in certain pronounced manners and show how to use them to identify the full or partial regularization of LSQR in practice.

**THEOREM 5.1.** *With the notation defined previously, the following results hold:*

$$(5.1) \quad \alpha_{k+1} < \gamma_k \leq \sqrt{1 + \eta_k^2 \sigma_{k+1}}, \quad k = 1, 2, \dots, n-1,$$

$$(5.2) \quad \beta_{k+2} < \gamma_k \leq \sqrt{1 + \eta_k^2 \sigma_{k+1}}, \quad k = 1, 2, \dots, n-1,$$

$$(5.3) \quad \alpha_{k+1} \beta_{k+2} \leq \frac{\gamma_k^2}{2} \leq \frac{(1 + \eta_k^2) \sigma_{k+1}^2}{2}, \quad k = 1, 2, \dots, n-1,$$

$$(5.4) \quad \gamma_{k+1} < \gamma_k, \quad k = 1, 2, \dots, n-2.$$

*Proof.* From (4.27), since  $P$  and  $Q_n$  are orthogonal matrices, we have

$$(5.5) \quad \gamma_k = \|A - P_{k+1} B_k Q_k^T\| = \|P^T (A - P_{k+1} B_k Q_k^T) Q_n\|$$

$$(5.6) \quad = \left\| \begin{pmatrix} B_n \\ \mathbf{0} \end{pmatrix} - (I, \mathbf{0})^T B_k (I, \mathbf{0}) \right\| = \|G_k\|$$

with

$$(5.7) \quad G_k = \begin{pmatrix} \alpha_{k+1} & & & & \\ \beta_{k+2} & \alpha_{k+2} & & & \\ & \beta_{k+3} & \ddots & & \\ & & \ddots & \alpha_n & \\ & & & \beta_{n+1} & \end{pmatrix} \in \mathbb{R}^{(n-k+1) \times (n-k)}$$

resulting from deleting the  $(k+1) \times k$  leading principal matrix of  $B_n$  and the first  $k$  zero rows and columns of the resulting matrix. From the above, for  $k = 1, 2, \dots, n-1$  we have

$$(5.8) \quad \alpha_{k+1}^2 + \beta_{k+2}^2 = \|G_k e_1\|^2 \leq \|G_k\|^2 = \gamma_k^2,$$

which shows that  $\alpha_{k+1} < \gamma_k$  and  $\beta_{k+2} < \gamma_k$  since  $\alpha_{k+1} > 0$  and  $\beta_{k+2} > 0$ . So from (4.2), we get (5.1) and (5.2). On the other hand, noting that

$$2\alpha_{k+1} \beta_{k+2} \leq \alpha_{k+1}^2 + \beta_{k+2}^2 \leq \gamma_k^2,$$

we get (5.3).

Note that  $\alpha_k > 0$  and  $\beta_{k+1} > 0$ ,  $k = 1, 2, \dots, n$ . By  $\gamma_k = \|G_k\|$  and (5.7), note that  $\gamma_{k+1} = \|G_{k+1}\|$  equals the 2-norm of the submatrix deleting the first column of

$G_k$ . Applying the Cauchy's strict interlacing theorem to the singular values of this submatrix and  $G_k$ , we obtain (5.4).  $\square$

REMARK 5.1. *For severely and moderately ill-posed problems, based on the results in the last section, (5.1) and (5.2) show that  $\alpha_{k+1}$  and  $\beta_{k+2}$  decay as fast as  $\sigma_{k+1}$  for  $k \leq k_0$  and their decays may become slow for  $k > k_0$ . For mildly ill-posed problems, since  $\eta_k$  are generally bigger than one considerably for  $k \leq k_0$ ,  $\alpha_{k+1}$  and  $\beta_{k+2}$  cannot generally decay as fast as  $\sigma_{k+1}$ , and their decays become slower for  $k > k_0$ .*

Gazzola and his coauthors [31, 35] claim without rigorous proofs that  $\alpha_{k+1}\beta_{k+1} = \mathcal{O}(k\sigma_k^2)$  and  $\alpha_{k+1}\beta_{k+2} = \mathcal{O}(k\sigma_{k+1}^2)$  for severely ill-posed problems with the constants in  $\mathcal{O}(\cdot)$  unknown (see Proposition 4 of [35]), but they do not show how fast each of them decays; see Proposition 6 of [35]. In contrast, our (5.1), (5.2) and (5.3) are rigorous and quantitative for all three kinds of ill-posed problems. In [36, Corollary 3.1], the authors have derived the product inequality

$$\prod_{k=1}^l \alpha_{k+1}\beta_{k+1} \leq \prod_{k=1}^l \sigma_k^2, \quad l = 1, 2, \dots, n-1.$$

Whether or not this inequality is sharp is unknown, as they point out. By it, they empirically claim that  $\alpha_{k+1}\beta_{k+1}$  may decay as fast as  $\sigma_k^2$  when the inequality is sharp; conversely, if it is not sharp, nothing can be said on how fast  $\alpha_{k+1}\beta_{k+1}$  decays.

We now shed light on (5.1) and (5.2). For a given (1.1), its degree of ill-posedness is either known or unknown. If it is unknown, (5.1) is of practical importance and can be exploited to identify whether or not LSQR has the full regularization without extra cost in an automatic and reliable way, so is (5.2). From the proofs of (5.1) and (5.2), we find that  $\alpha_{k+1}$  and  $\beta_{k+2}$  are as small as  $\gamma_k$ . Since our theory and analysis in Section 4 have proved that  $\gamma_k$  decays as fast as  $\sigma_{k+1}$  for severely or moderately ill-posed problems with  $\rho > 1$  or  $\alpha > 1$  suitably and it decays more slowly than  $\sigma_{k+1}$  for mildly ill-posed problems, the decay rate of  $\sigma_k$  can be judged by that of  $\alpha_k$  or  $\beta_{k+1}$  or better judged by that of  $\alpha_k + \beta_{k+1}$  reliably, as shown below.

Given (1.1), run LSQR until semi-convergence occurs at iteration  $k^*$ . Check how  $\alpha_k + \beta_{k+1}$  decays as  $k$  increases during the process. If, on average, it decays in an obviously exponential way, then (1.1) is a severely ill-posed problem. In this case, LSQR has the full regularization, and semi-convergence means that we have found a best possible regularized solution. If, on average,  $\alpha_k$  decays as fast as  $k^{-\alpha}$  with  $\alpha > 1$  considerably, then (1.1) is surely a moderately ill-posed problem, and LSQR also has found a best possible regularized solution at semi-convergence. If, on average, it decays at most as fast as or more slowly than  $k^{-\alpha}$  with  $\alpha$  no more than one, (1.1) is a mildly ill-posed problem. Notice that the noise  $e$  does not deteriorate regularized solutions until semi-convergence. Therefore, if a hybrid LSQR is used, then it is more reasonable and also cheaper to apply regularization to projected problems only from iteration  $k^* + 1$  onwards other than from the very start, i.e., the first iteration, as done in the hybrid Lanczos bidiagonalization/Tikhonov regularization scheme [8], until a best possible regularized solution is found. For a hybrid LSMR, regularization is applied to the projected problems generated in LSMR in the same way.

**5.2. The regularization of LSMR.** Based on the previous results, we can rigorously analyze the regularizing effects of LSMR [30, 11] and draw definitive conclusions on its regularization for three kinds of ill-posed problems.

LSMR is mathematically equivalent to MINRES applied to  $A^T A x = A^T b$ , and its iterate  $x_k^{lsmr}$  minimizes  $\|A^T(b - Ax)\|$  over  $x \in \mathcal{V}_k^R$ , and the residual norm  $\|A^T(b -$

$\|Ax_k^{lsmr}\|$  decreases monotonically with respect to  $k$ . In our notation, noting from Algorithm 1 that  $Q_{k+1}^T A^T A Q_k = (B_k^T B_k, \alpha_{k+1} \beta_{k+1} e_k)^T$  with rank  $k$ , it is known from Section 2.2 of [30] that

$$(5.9) \quad x_k^{lsmr} = Q_k y_k^{lsmr} = Q_k (Q_{k+1}^T A^T A Q_k)^\dagger Q_{k+1}^T A^T b,$$

which can be efficiently computed and updated. So LSMR amounts to solving the modified problem that perturbs the matrix  $A^T A$  in  $A^T A x = A^T b$  to its rank  $k$  approximation  $Q_{k+1} Q_{k+1}^T A^T A Q_k Q_k^T$ , and the iterate  $x_k^{lsmr}$  is the minimum-norm least squares solution to the modified problem

$$(5.10) \quad \min \|Q_{k+1} Q_{k+1}^T A^T A Q_k Q_k^T x - A^T b\|.$$

It is direct to verify that the TSVD solution  $x_k^{tsvd}$  is exactly the minimum-norm least squares solution to the modified problem  $\min \|A_k^T A_k x - A^T b\|$  that replaces  $A^T A$  by its 2-norm best rank  $k$  approximation  $A_k^T A_k$  in  $A^T A x = A^T b$ . As a result, the regularization problem for LSMR now becomes that of accurately estimating  $\|A^T A - Q_{k+1} Q_{k+1}^T A^T A Q_k Q_k^T\|$ , investigates how close it is to  $\sigma_{k+1}^2 = \|A^T A - A_k^T A_k\|$  and analyzes whether or not the singular values of  $Q_{k+1}^T A^T A Q_k$  approximate the  $k$  large singular values  $\sigma_i^2$ ,  $i = 1, 2, \dots, k$  of  $A^T A$  in natural order.

**THEOREM 5.2.** *For LSMR and  $k = 1, 2, \dots, n-1$ , we have*

$$(5.11) \quad \gamma_k^2 \leq \|A^T A - Q_{k+1} Q_{k+1}^T A^T A Q_k Q_k^T\| \leq \sqrt{1 + m_k (\gamma_{k-1}/\gamma_k)^2} \gamma_k^2$$

with  $0 \leq m_k < 1$ .

*Proof.* For the orthogonal matrix  $Q_n$  generated by Algorithm 1, noticing that  $\alpha_{n+1} = 0$ , from (2.1) and (2.2) we obtain  $Q_n^T A^T A Q_n = B_n^T B_n$  and

$$\begin{aligned} \|A^T A - Q_{k+1} Q_{k+1}^T A^T A Q_k Q_k^T\| &= \|Q_n^T (A^T A - Q_{k+1} Q_{k+1}^T A^T A Q_k Q_k^T) Q_n\| \\ &= \|B_n^T B_n - (I, \mathbf{0})^T (B_k^T B_k, \alpha_{k+1} \beta_{k+1} e_k)^T (I, \mathbf{0})\| \\ &= \|F_k\|, \end{aligned}$$

where  $F_k$  is the  $(n-k+1) \times (n-k)$  matrix that is generated by deleting the  $(k+1) \times k$  leading principal matrix of the symmetric tridiagonal matrix  $B_n^T B_n$  and the first  $k-1$  zero rows and  $k$  zero columns of the resulting matrix. Note that  $B_n^T B_n$  has the diagonals  $\alpha_k^2 + \beta_{k+1}^2$ ,  $k = 1, 2, \dots, n$  and the super- and sub-diagonals  $\alpha_k \beta_k$ ,  $k = 2, 3, \dots, n$ . We have

$$(5.12) \quad F_k = \begin{pmatrix} \alpha_{k+1} \beta_{k+1} & & & & & \\ \alpha_{k+1}^2 + \beta_{k+2}^2 & \alpha_{k+2} \beta_{k+2} & & & & \\ \alpha_{k+2} \beta_{k+2} & \alpha_{k+2}^2 + \beta_{k+3}^2 & \ddots & & & \\ & \alpha_{k+3} \beta_{k+3} & \ddots & & & \\ & & & \alpha_{n-1} \beta_{n-1} & & \\ & & & \ddots & \alpha_n^2 + \beta_n^2 & \alpha_n \beta_n \\ & & & & \alpha_n \beta_n & \alpha_n^2 + \beta_{n+1}^2 \end{pmatrix}$$

According to (5.7), it is direct to check that the  $(n-k) \times (n-k)$  symmetric tridiagonal matrix  $G_k^T G_k$  is a submatrix of  $F_k$  that deletes its first row  $\alpha_{k+1} \beta_{k+1} e_1^T$ . Therefore, we have  $\|F_k\| \geq \|G_k^T G_k\| = \|G_k\|^2 = \gamma_k^2$  with the last equality being from (5.5) and (5.6), which proves the lower bound in (5.11).



On the other hand, noting the strict inequalities in (5.1) and (5.2), since

$$F_k^T F_k = (G_k^T G_k)^2 + \alpha_{k+1}^2 \beta_{k+1}^2 e_1 e_1^T,$$

from [121, p.98] we obtain

$$\|F_k\|^2 = \|G_k\|^4 + m'_k \alpha_{k+1}^2 \beta_{k+1}^2 \leq \gamma_k^4 + m_k \gamma_{k-1}^2 \gamma_k^2$$

with  $0 \leq m'_k \leq 1$  and  $0 \leq m_k < m'_k$  if  $m'_k > 0$ , from which the upper bound of (5.11) follows directly.  $\square$

Recall that LSQR is mathematically equivalent to CGLS that implicitly applies the CG method to  $A^T A x = A^T b$ . By (2.6), (2.1), (2.2) and (2.4), noting that  $P_{k+1} P_{k+1}^T b = b$ , we obtain the LSQR iterates

$$\begin{aligned} x^{(k)} &= Q_k B_k^\dagger P_{k+1}^T b = Q_k (B_k^T B_k)^{-1} B_k^T P_{k+1}^T b \\ &= Q_k (Q_k^T A^T A Q_k)^{-1} Q_k^T A^T P_{k+1} P_{k+1}^T b = Q_k (Q_k^T A^T A Q_k)^{-1} Q_k^T A^T b, \end{aligned}$$

which is the minimum-norm least squares solution to the modified problem

$$(5.13) \quad \min \|Q_k Q_k^T A^T A Q_k Q_k^T x - A^T b\|$$

that replaces  $A^T A$  by its rank  $k$  approximation  $Q_k Q_k^T A^T A Q_k Q_k^T = Q_k B_k^T B_k Q_k^T$  in  $A^T A x = A^T b$ . As a result, in the sense of solving  $A^T A x = A^T b$ , for LSQR, the accuracy of such rank  $k$  approximation is  $\|A^T A - Q_k Q_k^T A^T A Q_k Q_k^T\|$ . We can establish the following result which relates the corresponding approximation accuracy concerning LSMR to that concerning LSQR.

**THEOREM 5.3.** *For the rank  $k$  approximations to  $A^T A$  defined in (5.10) and (5.13) involved in LSMR and LSQR, we have*

$$(5.14) \quad \|A^T A - Q_{k+1} Q_{k+1}^T A^T A Q_k Q_k^T\| \leq \|A^T A - Q_k Q_k^T A^T A Q_k Q_k^T\|.$$

*Proof.* Similar to the proof of Theorem 5.2, it is direct to verify that

$$\begin{aligned} \|A^T A - Q_k Q_k^T A^T A Q_k Q_k^T\| &= \|Q_n^T (A^T A - Q_k Q_k^T A^T A Q_k Q_k^T) Q_n\| \\ &= \|B_n^T B_n - (I, \mathbf{0})^T B_k^T B_k (I, \mathbf{0})\| \\ &= \|F'_k\|, \end{aligned}$$

where  $F'_k$  is an  $(n-k+1) \times (n-k+1)$  matrix whose first column is  $(0, \alpha_{k+1} \beta_{k+1}, \mathbf{0})^T$  and last  $n-k$  columns are just the matrix  $F_k$  defined by (5.12). Therefore, we have  $\|F_k\| \leq \|F'_k\|$ , which is just (5.3).  $\square$

This theorem indicates that, as far as solving  $A^T A x = A^T b$  is concerned, the rank  $k$  approximation in LSMR is at least as accurate as that in LSQR. However, regarding LSQR applied to (1.1) directly, Theorem 4.1 is much more attractive since it not only deals with the rank  $k$  approximation to  $A$  directly but also estimates the accuracy of the rank  $k$  approximation in terms of  $\sigma_{k+1}$  more compactly and informatively.

**REMARK 5.2.** *According to the results and analysis in Section 4, we have  $\gamma_{k-1}/\gamma_k \sim \rho$  for severely ill-posed problems, and  $\gamma_{k-1}/\gamma_k \sim (k/(k-1))^\alpha$  at most for moderately and mildly ill-posed problems. In comparison with Theorem 4.1, noting the form of the lower and upper bounds of (5.11), we see that  $Q_{k+1} Q_{k+1}^T A^T A Q_k Q_k^T =$*



$Q_{k+1}(B_k^T B_k, \alpha_{k+1}\beta_{k+1}e_k)^T Q_k^T$  as a rank  $k$  approximation to  $A^T A$  is basically as accurate as  $P_{k+1}B_k Q_k^T$  as a rank  $k$  approximation to  $A$ .

REMARK 5.3. From [109, p.33], the singular values of  $(B_k^T B_k, \alpha_{k+1}\beta_{k+1}e_k)^T$  are correspondingly bigger than those of  $B_k^T B_k$ , i.e.,  $(\theta_i^{(k)})^2$ . Therefore, the smallest singular value of  $(B_k^T B_k, \alpha_{k+1}\beta_{k+1}e_k)^T$  is no less than  $(\theta_k^{(k)})^2$ . As a result,  $(B_k^T B_k, \alpha_{k+1}\beta_{k+1}e_k)^T$  has no singular values smaller than  $\sigma_{k_0+1}^2$  before  $k \leq k_0$ , provided that  $\theta_k^{(k)} > \sigma_{k_0+1}$  for  $k \leq k_0$ . This means that the noise deteriorates the iterates  $x_k^{\text{lsmr}}$  no sooner than it does for the LSQR iterates  $x^{(k)}$ .

REMARK 5.4. A combination of Theorem 5.3 and the above two remarks means that the regularizing effects of LSMR are highly competitive with and not inferior to those of LSQR for each kind of ill-posed problem under consideration. Consequently, from the theory of LSQR in Section 4, we conclude that LSMR has the full regularization for severely or moderately ill-posed problems with  $\rho > 1$  or  $\alpha > 1$  suitably. However, Theorem 5.2 indicates that LSMR generally has only the partial regularization for mildly ill-posed problems since  $\gamma_{k_0}$  is generally bigger than  $\sigma_{k_0+1}$  considerably; see Remark 4.4.

REMARK 5.5. We can define a near best rank  $k$  approximation to  $A^T A$  similar to (4.18). Based on (5.11), if, in LSMR, we simply take  $\|A^T A - Q_{k+1}Q_{k+1}^T A^T A Q_k Q_k^T\| = \gamma_k^2$  for the ease of presentation, we can establish an analog of Theorem 4.2 for LSMR. In the meantime, completely parallel to the proof of Theorem 4.3, we can also derive an analog of Theorem 4.3 for LSMR, in which the sufficient conditions on  $\eta_k$  that ensure that the singular values of  $(B_k^T B_k, \alpha_{k+1}\beta_{k+1}e_k)^T$  approximate the first  $k$  large singular values of  $A^T A$  in natural order are found to be

$$2 + \eta_k^2 < \left( \frac{k_0 + 1}{k_0} \right)^{2\alpha}, \quad k = 1, 2, \dots, k_0$$

for  $A$  with  $\sigma_i = \zeta i^{-\alpha}$ .

REMARK 5.6. Since LSMR and LSQR have similar regularizing effects for each kind of ill-posed problem, we can judge the full or partial regularization of LSMR by inspecting the decay rate of  $\alpha_k + \beta_{k+1}$  with respect to  $k$ , as has been done for LSQR,

In Section 4 we have interpreted LSQR as solving the modified problem that perturbs  $A$  in (1.1) to its rank  $k$  approximation  $P_{k+1}B_k Q_k^T$ . The regularization of LSQR then is up to the accuracy of such rank  $k$  approximation to  $A$  and how the  $k$  large singular values of  $A$  are approximated by the nonzero singular values of  $B_k$ . We will treat CGME in the same way later. It might be hopeful to treat LSMR in this preferable and more direct way. From (5.9), LSMR is also equivalent to computing the minimum-norm least squares solution to the modified problem

$$\min \| (Q_k(Q_{k+1}^T A^T A Q_k)^\dagger Q_{k+1}^T A^T)^\dagger x - b \|,$$

which perturbs  $A$  in (1.1) to its rank  $k$  approximation  $(Q_k(Q_{k+1}^T A^T A Q_k)^\dagger Q_{k+1}^T A^T)^\dagger$ . However, an analysis of such formulation appears intractable because there is no explicit way to remove two generalized inverses  $^\dagger$  in such rank  $k$  approximation, which makes it impossible to accurately estimate  $\|A - (Q_k(Q_{k+1}^T A^T A Q_k)^\dagger Q_{k+1}^T A^T)^\dagger\|$  in terms of  $\sigma_{k+1}$ .

**5.3. The other rank  $k$  approximations to  $A$  generated by Lanczos bidiagonalization and the regularization of CGME.** By (2.1) and (2.2), we get

$$\begin{aligned}
 P_{k+1}P_{k+1}^T A &= P_{k+1}(B_k Q_k^T + \alpha_{k+1} e_{k+1} q_{k+1}^T) \\
 &= P_{k+1}(B_k, \alpha_{k+1} e_{k+1}) Q_{k+1}^T \\
 (5.15) \quad &= P_{k+1} \bar{B}_k Q_{k+1}^T,
 \end{aligned}$$

where  $Q_{k+1} = (Q_k, q_{k+1})$ , and  $\bar{B}_k = (B_k, \alpha_{k+1} e_{k+1}) \in \mathbb{R}^{(k+1) \times (k+1)}$  is lower bidiagonal with rank  $k+1$ . Thus, it follows from [45, 47, 61] that CGME is the CG method applied to  $\min \|AA^T y - b\|$  and  $x = A^T y$ , where the  $k$ -th iterate  $x_k^{cgme}$  minimizes the error  $\|A^\dagger b - x\|$ , i.e.,  $\|x_{naive} - x\|$ , over  $x \in \mathcal{V}_k^R$ , and the error norm  $\|x_{naive} - x_k^{cgme}\|$  decreases monotonically with respect to  $k$ . By Lanczos bidiagonalization, it is known from [45, 47, 61] that  $x_k^{cgme} = Q_k y_k^{cgme}$  with  $y_k^{cgme} = \|b\| \bar{B}_{k-1}^{-1} e_1^{(k)}$  and the residual norm  $\|Ax_k^{cgme} - b\| = \beta_{k+1} |e_k^T y_k^{cgme}|$  with  $e_k$  the  $k$ -th canonical vector of dimension  $k$ . Noting that  $\|b\| e_1^{(k)} = P_k^T b$ , we have

$$(5.16) \quad x_k^{cgme} = Q_k \bar{B}_{k-1}^{-1} P_k^T b.$$

Therefore,  $x_k^{cgme}$  is the minimum-norm least squares solution to the modified problem that replaces  $A$  in (1.1) by its rank  $k$  approximation  $P_k \bar{B}_{k-1} Q_k^T = P_k P_k^T A$ .

**THEOREM 5.4.** *For the rank  $k+1$  approximation  $P_{k+1}P_{k+1}^T A$  and the rank  $k$  approximation in CGME, we have*

$$(5.17) \quad \|(I - P_{k+1}P_{k+1}^T)A\| \leq \gamma_k \leq \sqrt{1 + \eta_k^2 \sigma_{k+1}},$$

$$(5.18) \quad \gamma_k < \|A - P_k \bar{B}_{k-1} Q_k^T\| \leq \gamma_{k-1}.$$

*Proof.* Since  $P_{k+1}P_{k+1}^T(I - P_{k+1}P_{k+1}^T) = 0$ , we obtain

$$\begin{aligned}
 \gamma_k^2 &= \|A - P_{k+1}B_k Q_k^T\|^2 \\
 &= \|P_{k+1}P_{k+1}^T A - P_{k+1}B_k Q_k^T + (I - P_{k+1}P_{k+1}^T)A\|^2 \\
 &= \max_{\|y\|=1} \|((P_{k+1}P_{k+1}^T A - P_{k+1}B_k Q_k^T) + (I - P_{k+1}P_{k+1}^T)A)y\|^2 \\
 &= \max_{\|y\|=1} \|P_{k+1}P_{k+1}^T(P_{k+1}P_{k+1}^T A - P_{k+1}B_k Q_k^T)y + (I - P_{k+1}P_{k+1}^T)Ay\|^2 \\
 &= \max_{\|y\|=1} (\|P_{k+1}P_{k+1}^T(P_{k+1}P_{k+1}^T A - P_{k+1}B_k Q_k^T)y\|^2 + \|(I - P_{k+1}P_{k+1}^T)Ay\|^2) \\
 &= \max_{\|y\|=1} (\|P_{k+1}(P_{k+1}^T A - B_k Q_k^T)y\|^2 + \|(I - P_{k+1}P_{k+1}^T)Ay\|^2) \\
 &= \max_{\|y\|=1} (\|(P_{k+1}^T A - B_k Q_k^T)y\|^2 + \|(I - P_{k+1}P_{k+1}^T)Ay\|^2) \\
 &\geq \max_{\|y\|=1} \|(I - P_{k+1}P_{k+1}^T)Ay\|^2 \\
 &= \|(I - P_{k+1}P_{k+1}^T)A\|^2,
 \end{aligned}$$

which, together with (4.2), establishes (5.17).

From (5.15) and (5.17) we obtain

$$(5.19) \quad \|(I - P_{k+1}P_{k+1}^T)A\| = \|A - P_{k+1}\bar{B}_k Q_{k+1}^T\| \leq \gamma_k.$$

The upper bound of (5.18) is direct (5.19) and (5.4) by noting that

$$\|A - P_k \bar{B}_{k-1} Q_k^T\| = \|(I - P_k P_k^T)A\| \leq \gamma_{k-1}.$$

Along the proof path of Theorem 5.1, we obtain

$$\|A - P_k \bar{B}_{k-1} Q_k^T\| = \|(\beta_{k+1} e_1, G_k)\|$$

with  $G_k$  defined by (5.7). It is straightforward to justify that the singular values of  $G_k \in \mathbb{R}^{(n-k+1) \times (n-k)}$  strictly interlace those of  $(\beta_k e_1, G_k) \in \mathbb{R}^{(n-k+1) \times (n-k+1)}$  by noting that  $(\beta_{k+1} e_1, G_k)^T (\beta_{k+1} e_1, G_k)$  is an *unreduced* symmetric tridiagonal matrix, from which and  $\|G_k\| = \gamma_k$  (cf. (5.5) and (5.6)) the lower bound of (5.18) follows.  $\square$

By the definition (4.1) of  $\gamma_k$ , this theorem indicates that  $P_k \bar{B}_{k-1} Q_k^T$  is definitely a less accurate rank  $k$  approximation to  $A$  than  $P_{k+1} B_k Q_k^T$  in LSQR. Moreover, a combination of it and Theorem 4.1 indicates that  $P_k \bar{B}_{k-1} Q_k^T$  may never be a near best rank  $k$  approximation to  $A$  even for severely and moderately ill-posed problems because, unlike LSQR, there do not exist sufficient conditions on  $\rho > 1$  and  $\alpha > 1$  to meet this requirement. For mildly ill-posed problems, CGME generally has only the partial regularization since  $\gamma_k$  has been proved to be generally bigger than  $\sigma_{k+1}$  substantially and is rarely close to  $\sigma_{k+1}$ .

Next we consider the other issue that is as equally important as the rank  $k$  approximation in CGME: the behavior of the singular values of  $\bar{B}_{k-1}$ , which are denoted by  $\bar{\theta}_i^{(k-1)}$ ,  $i = 1, 2, \dots, k$  labeled in the decreasing order. Observe that  $\bar{B}_{k-1}$  consists of the first  $k$  rows of  $B_k$ . Since  $B_k B_k^T$  is an  $(k+1) \times (k+1)$  unreduced symmetric tridiagonal matrix, whose eigenvalues are  $(\theta_1^{(k)})^2, (\theta_2^{(k)})^2, \dots, (\theta_k^{(k)})^2, 0$ , and  $\bar{B}_{k-1} \bar{B}_{k-1}^T$  is the  $k \times k$  leading principal submatrix of  $B_k B_k^T$ , whose eigenvalues are  $(\bar{\theta}_1^{(k-1)})^2, (\bar{\theta}_2^{(k-1)})^2, \dots, (\bar{\theta}_k^{(k-1)})^2$ , by the strict interlacing property of eigenvalues, we obtain

$$(5.20) \quad \theta_1^{(k)} > \bar{\theta}_1^{(k-1)} > \theta_2^{(k)} > \bar{\theta}_2^{(k-1)} > \dots > \theta_k^{(k)} > \bar{\theta}_k^{(k-1)} > 0, \quad k = 1, 2, \dots, n.$$

On the other hand, note that  $\alpha_{n+1} = 0$  and  $\bar{\theta}_i^{(n)} = \theta_i^{(n)} = \sigma_i$ ,  $i = 1, 2, \dots, n$ , i.e., the singular values of  $\bar{B}_n$  are  $\sigma_1, \sigma_2, \dots, \sigma_n$  and zero, which is denoted by the dummy  $\sigma_{n+1} = 0$ . Since  $\bar{\theta}_{n+1}^{(n)} = \sigma_{n+1} = 0$  and the first  $k$  rows of  $\bar{B}_n$  are  $(\bar{B}_{k-1}, \mathbf{0}) \in \mathbb{R}^{k \times n}$ , whose singular values are  $\bar{\theta}_1^{(k-1)}, \dots, \bar{\theta}_k^{(k-1)}$ , by applying the strict interlacing property of singular values to  $(\bar{B}_{k-1}, \mathbf{0})$  and  $\bar{B}_n$ , for  $k = 1, 2, \dots, n-1$  we have

$$(5.21) \quad \sigma_{n+1-k+i} < \bar{\theta}_i^{(k-1)} < \sigma_i, \quad i = 1, 2, \dots, k,$$

from which it follows that

$$(5.22) \quad 0 < \bar{\theta}_k^{(k-1)} < \sigma_k.$$

(5.20) and (5.22) indicate that, unlike  $\theta_k^{(k)}$  that lies between  $\sigma_{k+1}$  and  $\sigma_k$  and approximates  $\sigma_k$  for severely or moderately ill-posed problems with  $\rho > 1$  or  $\alpha > 1$  suitably (cf. (4.25)), the lower bound for  $\bar{\theta}_k^{(k-1)}$  is simply zero, and there does not exist a better one for it. This means that  $\bar{\theta}_k^{(k-1)}$  may be much smaller than  $\sigma_{k_0+1}$  and actually it can be arbitrarily small, independently of the degree  $\rho$  or  $\alpha$  of ill-posedness. In other words, the size of  $\rho$  or  $\alpha$  does not have any intrinsic effects on the

lower bound of  $\bar{\theta}_k^{(k-1)}$ , and one thus cannot control  $\bar{\theta}_k^{(k-1)}$  from below by choosing  $\rho$  or  $\alpha$ . In the meantime, (5.20) tells us that  $\bar{\theta}_k^{(k-1)} < \theta_k^{(k)}$ . These facts, together with Theorem 5.4, show that the regularization of CGME is inferior to that of LSQR and LSMR for each kind of problem. On the one hand, they mean that CGME has the partial regularization for mildly ill-posed problems; on the other hand, the regularizing effects of CGME have indeterminacy for severely and moderately ill-posed problems, that is, it may or may not have the full regularization for these two kinds of problems. Clearly, CGME has the full regularization only when  $P_k \bar{B}_{k-1} Q_k^T$  is as accurate as the rank  $k$  approximation  $P_{k+1} B_k Q_k^T$  and  $\bar{\theta}_k^{(k-1)} \approx \theta_k^{(k)}$ ,  $k = 1, 2, \dots, k_0$  for these two kinds of problems with  $\rho > 1$  and  $\alpha > 1$  considerably, but unfortunately there is no guarantee that these requirements are satisfied mathematically.

The above analysis indicates that CGME itself is not reliable and cannot be trusted to compute best possible regularized solutions. In principle, one can detect the full or partial regularization of CGME as follows: One first exploits the decay rate of  $\alpha_k + \beta_{k+1}$  to identify the degree of ill-posedness of (1.1). If (1.1) is mildly ill-posed, CGME has only the partial regularization. If (1.1) is recognized as severely or moderately ill-posed, one then needs to do two things to identify the regularization of CGME: check if  $\|A - P_k \bar{B}_{k-1} Q_k\| \approx \|A - P_{k+1} B_k Q_k\|$ , and compute the singular values of both  $B_k$  and  $\bar{B}_{k-1}$  and check if  $\bar{\theta}_k^{(k-1)} \approx \theta_k^{(k)}$ . If both hold, CGME has the full regularization; if either of them does not hold, it has only the partial regularization.

We can informally deduce more features on CGME. For the LSQR iterate  $x^{(k)}$ , note that the optimality requirement of CGME means that  $\|x_{naive} - x_k^{cgme}\| \leq \|x_{naive} - x^{(k)}\|$ . Since

$$\|x_{naive} - x_k^{cgme}\| = \|x_{naive} - x_{true} + x_{true} - x_k^{cgme}\| \leq \|x_{naive} - x_{true}\| + \|x_{true} - x_k^{cgme}\|$$

and

$$\|x_{naive} - x^{(k)}\| = \|x_{naive} - x_{true} + x_{true} - x^{(k)}\| \leq \|x_{naive} - x_{true}\| + \|x_{true} - x^{(k)}\|$$

with the first terms in the right-hand sides being the same constant, not rigorously speaking, we should have

$$(5.23) \quad \|x_{true} - x_k^{cgme}\| \leq \|x_{true} - x^{(k)}\|$$

until the semi-convergence of CGME. Keep in mind that the regularization of CGME is inferior to or are at most as good as that of LSQR for each kind of ill-posed problem. Both  $\|x_{true} - x_k^{cgme}\|$  and  $\|x_{true} - x^{(k)}\|$  first decrease until their respective semi-convergence and then become increasingly large as  $k$  increases. As a result, we deduce that (i)  $x_k^{cgme}$  is at least as accurate as  $x^{(k)}$  until the semi-convergence of CGME and (ii) CGME reaches semi-convergence no later than LSQR; otherwise, (5.23) indicates that the optimal regularized solution by CGME at semi-convergence would be more accurate than that by LSQR at semi-convergence, which contradicts the property that LSQR has better regularization than CGME. The experiments in [47] justify this assertion; see Figure 3.1 and Figure 5.2 there.

Next let us return to (5.19) and show how to extract a rank  $k$  approximation to  $A$  from the rank  $k+1$  approximation  $P_{k+1} \bar{B}_k Q_{k+1}^T$  as best as possible.

**THEOREM 5.5.** *Let  $\bar{C}_k$  be the best rank  $k$  approximation to  $\bar{B}_k$  with respect to the 2-norm. Then*

$$(5.24) \quad \|A - P_{k+1} \bar{C}_k Q_{k+1}^T\| \leq \sigma_{k+1} + \gamma_k,$$

$$(5.25) \quad \|A - P_{k+1} \bar{C}_k Q_{k+1}^T\| \leq \bar{\theta}_{k+1}^{(k)} + \gamma_k,$$

where  $\bar{\theta}_{k+1}^{(k)}$  is the smallest singular value of  $\bar{B}_k$ .

*Proof.* Write  $A - P_{k+1}\bar{C}_kQ_{k+1}^T = A - P_{k+1}\bar{B}_kQ_{k+1}^T + P_{k+1}(\bar{B}_k - \bar{C}_k)Q_{k+1}^T$ . Then from (5.15) we obtain

$$(5.26) \quad \|A - P_{k+1}\bar{C}_kQ_{k+1}^T\| \leq \|A - P_{k+1}\bar{B}_kQ_{k+1}^T\| + \|P_{k+1}(\bar{B}_k - \bar{C}_k)Q_{k+1}^T\|$$

$$(5.27) \quad = \|A - P_{k+1}\bar{B}_kQ_{k+1}^T\| + \|P_{k+1}P_{k+1}^T A - P_{k+1}\bar{C}_kQ_{k+1}^T\|.$$

By the assumption on  $C_k$  and (5.15),  $P_{k+1}\bar{C}_kQ_{k+1}^T$  is the best rank  $k$  approximation to  $P_{k+1}\bar{B}_kQ_{k+1}^T = P_{k+1}P_{k+1}^T A$ . Keep in mind that  $A_k$  is the best rank  $k$  approximation to  $A$ . Since  $P_{k+1}P_{k+1}^T A_k$  is a rank  $k$  approximation to  $P_{k+1}P_{k+1}^T A$ , we get

$$\begin{aligned} \|P_{k+1}P_{k+1}^T A - P_{k+1}\bar{C}_kQ_{k+1}^T\| &\leq \|P_{k+1}P_{k+1}^T (A - A_k)\| \\ &\leq \|A - A_k\| = \sigma_{k+1}, \end{aligned}$$

from which, (5.19) and (5.27) it follows that (5.24) holds.

Since  $P_{k+1}$  and  $Q_{k+1}$  are orthonormal, by the 2-norm invariance, we obtain

$$\|P_{k+1}(\bar{B}_k - \bar{C}_k)Q_{k+1}^T\| = \|\bar{B}_k - \bar{C}_k\| = \bar{\theta}_{k+1}^{(k)},$$

from which and (5.26) it follows that (5.25) holds.  $\square$

We point out that (5.24) may be conservative since we have amplified  $\|P_{k+1}(\bar{B}_k - \bar{C}_k)Q_{k+1}^T\|$  twice and obtained its bound  $\sigma_{k+1}$ , which can be a considerable overestimate. In comparison with (4.1) and (4.2), the bound (5.24) indicates that  $P_{k+1}\bar{C}_kQ_{k+1}^T$  may not be as accurate as  $P_{k+1}B_kQ_k^T$ , but (5.25) illustrates that  $P_{k+1}\bar{C}_kQ_{k+1}^T$  can be as accurate as  $P_{k+1}B_kQ_k^T$  because  $\bar{\theta}_{k+1}^{(k)} < \theta_{k+1}^{(k+1)} < \sigma_{k+1}$  from (5.20) and (4.25). Moreover, as we have explained,  $\bar{\theta}_{k+1}^{(k)}$  can be arbitrarily small. If so,  $\bar{\theta}_{k+1}^{(k)}$  is negligible in (5.25) and  $P_{k+1}\bar{C}_kQ_{k+1}^T$  is at least as accurate as  $P_{k+1}B_kQ_k^T$ .

We now present a new but informal analysis to show why  $P_{k+1}\bar{C}_kQ_{k+1}^T$  may be at least as accurate as  $P_{k+1}B_kQ_k^T$  as a rank  $k$  approximation to  $A$ . Keep in mind that  $\bar{\theta}_i^{(k)}$ ,  $i = 1, 2, \dots, k+1$  be the singular values of  $\bar{B}_k$ . Then the singular values of  $\bar{C}_k$  are  $\bar{\theta}_i^{(k)}$ ,  $i = 1, 2, \dots, k$ . Since  $\alpha_{k+1} > 0$  for  $k \leq n-1$ , applying the strict interlacing property of singular values to  $B_k$  and  $\bar{B}_k$ , we have

$$(5.28) \quad \bar{\theta}_1^{(k)} > \theta_1^{(k)} > \bar{\theta}_2^{(k)} > \dots > \bar{\theta}_k^{(k)} > \theta_k^{(k)} > \bar{\theta}_{k+1}^{(k)} > 0, \quad k = 1, 2, \dots, n-1.$$

The above relationships, together with (4.29), prove that

$$(5.29) \quad \sigma_i - \bar{\theta}_i^{(k)} < \sigma_i - \theta_i^{(k)} \leq \gamma_k, \quad i = 1, 2, \dots, k,$$

that is, the  $\bar{\theta}_i^{(k)}$  are more accurate than  $\theta_i^{(k)}$  as approximations to  $\sigma_i$ ,  $i = 1, 2, \dots, k$ . By the standard perturbation theory, note from (5.19) that

$$\sigma_i - \bar{\theta}_i^{(k)} \leq \|A - P_{k+1}\bar{B}_kQ_{k+1}^T\| \leq \gamma_k, \quad i = 1, 2, \dots, k+1,$$

while the singular value differences between  $A$  and  $P_{k+1}\bar{C}_kQ_{k+1}^T$  are  $\sigma_i - \bar{\theta}_i^{(k)}$ ,  $i = 1, 2, \dots, k$  and  $\sigma_i$ ,  $i = k+1, \dots, n$ , all of which, from (5.29) and (4.2), are no more than  $\gamma_k$ . Based on these rigorous facts and the relationship between  $C_k$  and  $\bar{B}_k$ , it is possible that  $\|A - P_{k+1}\bar{C}_kQ_{k+1}^T\| \leq \gamma_k$ , and if it is so, then by definition (4.1)  $P_{k+1}\bar{C}_kQ_{k+1}^T$  is a more accurate rank  $k$  approximation to  $A$  than  $P_{k+1}B_kQ_k^T$  is.

**5.4. A comparison with standard randomized algorithms and RRQR factorizations.** We compare the rank approximations  $P_{k+1}B_kQ_k^T$  and  $P_{k+1}\bar{C}_kQ_{k+1}^T$  by Lanczos bidiagonalization with those by some standard randomized algorithms and RRQR factorizations, and demonstrate that the former ones are much more accurate than the latter ones for severely and moderately ill-posed problems.

Note (4.5). Compare (4.2), (5.17) and (5.24) or (5.25) with the corresponding results (1.9), (5.6), (6.3) and Theorem 9.3 in [43] for standard randomized algorithms and those on the strong RRQR factorization [42], where the constants in front of  $\sigma_{k+1}$  are like  $\sqrt{kn}$  and  $\sqrt{1+4k(n-k)}$ , respectively, which are far bigger than one. Within the framework of the RRQR factorizations, it is known from [63] that the optimal factor of such kind is  $\sqrt{k(n-k)+\min\{k, n-k\}}$  but to find corresponding permutations is an NP-hard problem, whose cost increases exponentially with  $n$ ; see also [11, p.298]. Clearly, the strong RRQR factorizations are near-optimal within the framework, and they suit well for finding a high quality low rank  $k$  approximation to a matrix whose  $k$  large singular values are much bigger than the  $n-k$  small ones.

Unfortunately, the standard randomized algorithms and RRQR factorization do not very nicely fit into solving ill-posed problems: they have regularizing effects but, in general, cannot find best possible regularized solutions. We argue as follows: Since there are no considerable gaps of singular values, the RRQR factorization techniques can hardly find a near best rank  $k$  approximation to  $A$  in the sense of (4.18), which is vital to solve (1.1) to find a best possible regularized solution. In contrast, for a severely or moderately ill-posed problem with  $\rho > 1$  or  $\alpha > 1$  suitably, the rank  $k$  approximations  $P_{k+1}B_kQ_k^T$  are near best ones for  $k = 1, 2, \dots, k_0$  and no singular value smaller than  $\sigma_{k_0+1}$  appears. Besides, it is easy to check that the  $k$ -step Lanczos bidiagonalization costs fewer flops than the standard randomized algorithms do for a sparse  $A$ , and it is more efficient than the strong RRQR factorization for a dense  $A$ , which includes  $\mathcal{O}(mnk)$  flops and the overhead cost of searching permutations.

For further developments and recent advances on randomized algorithms, we refer to Gu's work [41], where he has considered randomized algorithms within the subspace iteration framework proposed in [43], presented a number of new results and improved the error bounds for the rank  $k$  approximations that are iteratively extracted. Such approaches may be promising to solve ill-posed problems.

## 6. The filters $f_i^{(k)}$ and a comparison of LSQR and the TSVD method.

Based on Proposition 3.1, exploiting Theorem 4.1, Theorem 4.3 and Theorem 5.1, we present the following results, which, from the viewpoint of Tikhonov regularization, explain why LSQR has the full regularization for severely and moderately ill-posed problems with  $\alpha > 1$  and  $\alpha > 1$  suitably and why it generally has the partial regularization for mildly ill-posed problems.

**THEOREM 6.1.** *For the severely or moderately ill-posed problems with  $\rho > 1$  or  $\alpha > 1$ , under the assumptions of Theorem 4.3, let  $f_i^{(k)}$  be defined by (3.2). Then for  $k = 1, 2, \dots, k_0$  we have*

$$(6.1) \quad |f_i^{(k)} - 1| \approx \frac{2\sigma_{k+1}}{\sigma_i} \left| \prod_{j=1, j \neq i}^k \left( 1 - \left( \frac{\sigma_i}{\sigma_j} \right)^2 \right) \right|, \quad i = 1, 2, \dots, k,$$

$$(6.2) \quad f_i^{(k)} \approx \sigma_i^2 \sum_{j=1}^k \frac{1}{\sigma_j^2}, \quad i = k+1, k+2, \dots, n.$$

*Proof.* For  $k = 1, 2, \dots, k_0$ , it follows from (3.2) that

$$|f_i^{(k)} - 1| = \left| \frac{(\theta_i^{(k)})^2 - \sigma_i^2}{(\theta_i^{(k)})^2} \prod_{j=1, j \neq i}^k \frac{(\theta_j^{(k)})^2 - \sigma_i^2}{(\theta_j^{(k)})^2} \right|, \quad i = 1, 2, \dots, k.$$

To simplify presentations and illuminate the essence, for the severely and moderately ill-posed problems with  $\rho > 1$  and  $\alpha > 1$  suitably, we simply replace  $\sqrt{1 + \eta_k^2}$  in (4.23) by one. On the other hand, we replace the denominator of  $\frac{(\theta_i^{(k)})^2 - \sigma_i^2}{(\theta_i^{(k)})^2}$  by  $\sigma_i^2$ . Then by (4.23) we approximately have

$$\sigma_i^2 - (\theta_i^{(k)})^2 = (\sigma_i - \theta_i^{(k)})(\sigma_i + \theta_i^{(k)}) \approx 2\sigma_{k+1}\sigma_i.$$

For  $j = 1, 2, \dots, k$  but  $i$ , replace  $\theta_j^{(k)}$  by  $\sigma_j$  approximately. Then (6.1) follows.

By (4.25), since  $\theta_k^{(k)} > \sigma_i$  for  $i = k+1, \dots, n$ , the factors  $\sigma_i/\theta_j^{(k)} < 1$  and decay to zero with increasing  $i$  for each fixed  $j \leq k$ . Therefore, for  $i = k+1, \dots, n$  we get

$$\begin{aligned} f_i^{(k)} &= 1 - \prod_{j=1}^k \left( 1 - \left( \frac{\sigma_i}{\theta_j^{(k)}} \right)^2 \right) \\ &= 1 - \left( 1 - \sum_{j=1}^k \left( \frac{\sigma_i}{\theta_j^{(k)}} \right)^2 \right) + \mathcal{O} \left( \frac{\sigma_i^4}{(\theta_{k-1}^{(k)} \theta_k^{(k)})^2} \right) \\ &= \sum_{j=1}^k \left( \frac{\sigma_i}{\theta_j^{(k)}} \right)^2 + \mathcal{O} \left( \frac{\sigma_i^4}{(\theta_{k-1}^{(k)} \theta_k^{(k)})^2} \right) \end{aligned}$$

Replace  $\theta_j^{(k)}$  by its upper bound  $\sigma_j$ ,  $j = 1, 2, \dots, k$  in the above, and note that the second term is higher order small relative to the first term. Then (6.2) follows.  $\square$

REMARK 6.1. For  $k = 1, 2, \dots, k_0$ , since  $\sigma_i$ ,  $i = 1, 2, \dots, k$  are dominant singular values, the factors

$$\left| \prod_{j=1, j \neq i}^k \left( 1 - \left( \frac{\sigma_i}{\sigma_j} \right)^2 \right) \right|, \quad i = 1, 2, \dots, k,$$

are modest. Consequently, (6.1) indicates that the  $f_i^{(k)} \approx 1$  with the errors  $\mathcal{O}(\sigma_{k+1}/\sigma_i)$  for  $i = 1, 2, \dots, k$ , while (6.2) shows that the  $f_i^{(k)}$  are at least as small as  $\sigma_i^2/\sigma_k^2$  for  $i = k+1, \dots, n$  and decrease with increasing  $i$ .

REMARK 6.2. For mildly ill-posed problems and  $k = 1, 2, \dots, k_0$ , as we have shown in Remark 3.12 and Section 4, it is generally the case that  $\theta_k^{(k)} < \sigma_{k_0+1}$ . Suppose  $\theta_k^{(k)} > \sigma_{j^*}$  with the smallest integer  $j^* > k_0 + 1$ . Then we have shown in the paragraph after Proposition 3.1 that  $f_i^{(k)} \geq 1$ ,  $i = k_0 + 1, \dots, j^* - 1$ . As a result, LSQR has only the partial regularization.

Recall that  $\Delta_k = (\delta_1, \delta_2, \dots, \delta_k)$ , and define  $U_k^o = (u_{k+1}, \dots, u_n)$ . In terms of (3.20)–(3.22), Hansen [53, p.151,155, Theorems 6.4.1-2] presents the following bounds

$$(6.3) \quad |f_i^{(k)} - 1| \leq \frac{\sigma_{k+1}}{\sigma_i} \frac{(\|(U_k^o)^T b\| + \sigma_{k+1} \|\Delta_k\| \|x^{(k)}\|) \|\delta_i\|}{|u_i^T b|}, \quad i = 1, 2, \dots, k,$$



$$(6.4) \quad \|\delta_i\|_\infty \leq \frac{\sigma_{k+1}}{\sigma_i} \frac{|u_{k+1}^T b|}{|u_i^T b|} |L_i^{(k)}(0)|, \quad i = 1, 2, \dots, k,$$

and

$$(6.5) \quad 0 \leq f_i^{(k)} \leq \frac{\sigma_i^2}{\sigma_k^2} |L_k^{(k)}(0)| \sum_{j=1}^k f_j^{(k)}, \quad i = k+1, \dots, n,$$

where  $\|\cdot\|_\infty$  is the infinity norm of a vector.

We now address a few points on the bounds (6.3) and (6.5). First, there had no estimates for  $\|\Delta_k\|$  and  $|L_i^{(k)}(0)|$ ,  $i = 1, 2, \dots, k$ ; second, what we need is  $\|\delta_k\|$  other than  $\|\delta_k\|_\infty$ , and as is seen from its proof in [53, p.151], it is relatively easy to obtain the accurate bound (6.4) for  $\|\delta_i\|_\infty$ , whereas it is hard to derive an accurate one for  $\|\delta_i\|$ . Because of lacking accurate estimates, it is unclear how small or large the bound (6.3) and (6.5) are. Moreover, as it will appear soon, the factor  $\sigma_{k+1} \|(U_k^o)^T b\|$  in the numerator of (6.3) may be a too crude overestimate, such that the bound (6.3) is pessimistic and is useless to estimate  $|f_i^{(k)} - 1|$ ,  $i = 1, 2, \dots, k$  and  $f_i^{(k)}$ ,  $i = k+1, \dots, n$ . Let us have a closer look at these points. Obviously, exploiting (6.4), we can only obtain the bounds

$$\begin{aligned} \|\delta_i\|_\infty &\leq \|\delta_i\| \leq \sqrt{n-k} \|\delta_i\|_\infty, \\ \max_{i=1,2,\dots,k} \|\delta_i\| &\leq \|\Delta_k\| \leq \sqrt{k} \max_{i=1,2,\dots,k} \|\delta_i\|, \end{aligned}$$

from which it follows that

$$\max_{i=1,2,\dots,k} \|\delta_i\|_\infty \leq \|\Delta_k\| \leq \sqrt{k(n-k)} \max_{i=1,2,\dots,k} \|\delta_i\|_\infty.$$

As a result, the estimates for both  $\|\delta_i\|$  and  $\|\Delta_k\|$  are too crude for  $n$  large and  $k$  small. Indeed, as we have seen previously, their accurate estimates are much involved and complicated. In Theorem 3.5, we have derived accurate estimates for  $\|\delta_i\|$ ,  $i = 1, 2, \dots, k$ ; see (3.53), (3.54) for severely ill-posed problems and (3.56), (3.57) for moderately and mildly ill-posed problems. Theorems 3.1–3.3 have given sharp estimates for  $\|\Delta_k\|$  for three kinds of problems, respectively.

The factor  $\sigma_{k+1} \|(U_k^o)^T b\|$  itself in the numerator of (6.3), though simple and elegant in form, does not give clear and quantitative information on its size. As a matter of fact, one must analyze its size carefully for the two cases  $k \leq k_0$  and  $k > k_0$ , respectively, for each kind of ill-posed problem; see the discrete Picard condition (1.6) and (1.7). For each of these two cases, using our proof approach used for Theorems 3.1, 3.3 and 3.5, we can obtain accurate estimates for  $\|(U_k^o)^T b\| = \left( \sum_{j=k+1}^n |u_j^T b|^2 \right)^{1/2}$  for three kinds of ill-posed problems, respectively. However, the point is that the factor  $\sigma_{k+1} \|(U_k^o)^T b\|$  results from a substantial amplification in the derivation. It is seen from the last line of [53, p.155] that this factor results from simply bounding it by

$$\|\Sigma_k^\perp (U_k^{(o)})^T b\| \leq \sigma_{k+1} \|(U_k^{(o)})^T b\|,$$

where  $\Sigma_k^\perp = \text{diag}(\sigma_{k+1}, \dots, \sigma_n)$ . For our context, this amplification is fatal, and it is subtle to obtain sharp bounds for  $\|\Sigma_k^\perp (U_k^{(o)})^T b\|$ . We observe that  $\|\Sigma_k^\perp (U_k^{(o)})^T b\|$



is nothing but the first square root factor in (3.19), for which we have established the accurate estimates (3.23) and (3.39) for severely, moderately and mildly ill-posed problems, respectively, which hold for  $k = 1, 2, \dots, n-1$  and are *independent* of  $n$ . It can be checked that these bounds for  $\|\Sigma_k^\perp (U_k^{(o)})^T b\|$  are substantially smaller than  $\sigma_{k+1} \|(U_k^{(o)})^T b\|$ .

After the above substantial improvements on (6.3) and (6.5), we can exploit the accurate bounds for  $\|\Delta_k\|$  and  $\|\delta_i\|$  in Theorems 3.1–3.3 and Theorem 3.5, as well as the remarks on them, to accurately estimate the bounds (6.3) and (6.5). From them we can draw the full regularization LSQR for severely and moderately ill-posed problems with  $\rho > 1$  and  $\alpha > 1$  suitably and its partial regularization for mildly ill-posed problems.

Making use of some standard perturbation results from Hansen [56], we can quantitatively relate LSQR to the TSVD method and analyze the differences between their corresponding regularized solutions and differences between  $P_{k+1}B_kQ_k^T x^{(k)}$  and  $A_k x_k^{tsvd}$  predicting the right-hand side  $b$  for  $k = 1, 2, \dots, k_0$ .

**THEOREM 6.2.** *For the severely or moderately ill-posed problem (1.1), let  $A_k$  be the rank  $k$  best approximation to  $A$ , and assume that  $\|E_k\| = \|P_{k+1}B_kQ_k^T - A_k\| \leq \sigma_k - \sigma_{k+1}$ . Then for  $k = 1, 2, \dots, k_0$  we have*

$$(6.6) \quad \frac{\|x^{(k)} - x_k^{tsvd}\|}{\|x_k^{tsvd}\|} \leq \frac{\kappa(A_k)}{1 - \epsilon_k} \left( \frac{\|E_k\|}{\|A_k\|} + \frac{\epsilon_k}{1 - \epsilon_k - \hat{\epsilon}_k} \frac{\|A_k x_k^{tsvd} - b\|}{\|A_k x_k^{tsvd}\|} \right),$$

$$(6.7) \quad \frac{\|P_{k+1}B_kQ_k^T x^{(k)} - A_k x_k^{tsvd}\|}{\|b\|} \leq \frac{\epsilon_k}{1 - \epsilon_k},$$

where

$$\kappa(A_k) = \frac{\sigma_1}{\sigma_k}, \quad \epsilon_k = \frac{\|E_k\|}{\sigma_k}, \quad \hat{\epsilon}_k = \frac{\sigma_{k+1}}{\sigma_k}.$$

*Proof.* For the problem  $\min \|A_k x - b\|$  that replaces  $A$  by  $A_k$  in (1.1), we regard the rank  $k$  matrix  $P_{k+1}B_kQ_k^T$  as a perturbed  $A_k$  with the perturbation matrix  $E_k = P_{k+1}B_kQ_k^T - A_k$ . Then by the standard perturbation results on the TSVD solutions [56, p.65-6], we obtain (6.6) and (6.7) directly.  $\square$

**REMARK 6.3.** Write  $\|E_k\| = \|P_{k+1}B_kQ_k^T - A + A - A_k\|$ . Since the rank  $k$  matrices  $P_{k+1}B_kQ_k^T$  and  $A_k$  have the  $k$  nonzero singular values  $\theta_i^{(k)}$  and  $\sigma_i$ ,  $i = 1, 2, \dots, k$ , respectively, from Mirsky's theorem [109, p.204, Theorem 4.11] we get the bounds

$$(6.8) \quad \max_{i=1, \dots, k} |\sigma_i - \theta_i^{(k)}| \leq \|E_k\| = \|A_k - P_{k+1}B_kQ_k^T\|,$$

$$(6.9) \quad \max\{\max_{i=1, \dots, k} |\sigma_i - \theta_i^{(k)}|, \sigma_{k+1}\} \leq \|A - P_{k+1}B_kQ_k^T\| = \gamma_k,$$

where the lower bound in (6.8) is no more than the one in (6.9). It is then expected that  $\|E_k\| \leq \gamma_k \approx \sigma_{k+1}$  for severely and moderately ill-posed problems. Therefore, we have  $\epsilon_k \approx \hat{\epsilon}_k < 1$ , and (6.7) indicates that  $\|P_{k+1}B_kQ_k^T x^{(k)} - A_k x_k^{tsvd}\|$ , is basically no more than  $\epsilon_k$ ,  $k = 1, 2, \dots, k_0$ .

**REMARK 6.4.** From (6.6), since the possibly not small factor

$$\frac{\|A_k x_k^{tsvd} - b\|}{\|A_k x_k^{tsvd}\|}$$

enters the bound (6.6), two regularized solutions  $x^{(k)}$  and  $x_k^{tsvd}$  may differ considerably even though  $P_{k+1}B_kQ_k^T x^{(k)}$  and  $A_k x_k^{tsvd}$  predict the right-hand side  $b$  with similar accuracy for  $k = 1, 2, \dots, k_0$ . This is the case for the inconsistent ill-posed problem  $\min \|Ax - b\|$  with  $m > n$ , where  $\|A_k x_k^{tsvd} - b\|$  decreases with respect to  $k$  until

$$\|A_{k_0} x_{k_0}^{tsvd} - b\|^2 = \|A x_{k_0}^{tsvd} - b\|^2 \approx \frac{n - k_0}{m} \|e\|^2 + \|(I - U_n U_n^T)b\|^2,$$

with  $U_n$  the first  $n$  columns of the  $m \times m$  left singular vector matrix  $U$  and  $\|(I - U_n U_n^T)b\|$  the incompatible part of  $b$  lying outside of the range of  $A$  (cf. [56, p.71,88]). Here we remark that the term  $\|(I - U_n U_n^T)b\|$  appears in the relation (4.17) of [56, p.71] but is missing in the above right-hand side [56, p.88]. For the consistent  $Ax = b$ , since  $\|(I - U_n U_n^T)b\| = 0$ , the right-hand side of (6.6) is approximately

$$\frac{\sigma_{k_0+1}}{\sigma_{k_0}} \left( 1 + \frac{\sigma_1}{\sigma_{k_0}} \sqrt{\frac{n - k_0}{m}} \frac{\|e\|}{\|b\|} \right).$$

We see from the above and (6.7) that two different regularized solutions can be quite different even if their residual norms are of similar very sizes, as addressed by Hansen [53, p.123-4, Theorem 5.7.1]. However, we point out that the accuracy of different regularized solutions as approximations to  $x_{true}$  can be compared. If the norms of errors of them and  $x_{true}$  have very comparable sizes, they are equally accurate regularized solutions to (1.1).

REMARK 6.5. Note that  $\|E_k\| = \|P_{k+1}B_kQ_k^T - A_k\| \leq \sigma_k - \sigma_{k+1}$  is assumed only for severely and moderately ill-posed problems. As the previous analysis has indicated, we have  $\|E_k\| \approx \gamma_k \approx \sigma_{k+1}$ . As a result, it is easily justified that this assumption is valid for these two kinds of problems provided that  $\rho > 1$  and  $\alpha > 1$  suitably. However, the assumption fails to hold for the mildly ill-posed problems with  $\sigma_i = \zeta i^{-\alpha}$ ,  $i = 1, 2, \dots, n$  and  $\frac{1}{2} < \alpha \leq 1$  since, for  $k > 1$ , we have

$$\sigma_k - \sigma_{k+1} = \sigma_{k+1} \left( \left( \frac{k+1}{k} \right)^\alpha - 1 \right) < \sigma_{k+1} \leq \gamma_k \approx \|E_k\|.$$

**7. The extension to the case that  $A$  has multiple singular values.** Previously, under the assumption that the singular values of  $A$  are simple, we have proved the results and made a detailed analysis on them. Recall the basic fact that the singular values  $\theta_i^{(k)}$ ,  $i = 1, 2, \dots, k$  of  $B_k$  are always simple mathematically, independent of whether the singular values of  $A$  are simple or multiple. In other words, the Lanczos bidiagonalization process works as if the singular values of  $A$  are simple, and the Ritz values  $\theta_i^{(k)}$ ,  $i = 1, 2, \dots, k$ , are the approximations to some of the *distinct* singular values of  $A$ . In this section, we will show that, by making a number of suitable and nontrivial changes and reformulations, our previous results and analysis can be extended to the case that  $A$  has multiple singular values.

Assume that  $A$  has  $s$  distinct singular values  $\sigma_1 > \sigma_2 > \dots > \sigma_s > 0$  with  $\sigma_i$  being  $c_i$  multiple and  $s \leq n$ . In order to treat this case, we need to make a number of preliminary preparations and necessary modifications or reformulations. Below let us show the detail.

First of all, we need to take  $b$  into consideration and present a new form SVD of  $A$  by selecting a specific set of left and right singular vectors corresponding to a

multiple singular value  $\sigma_i$  of  $A$ , so that the discrete Picard condition (1.6) holds for one particularly chosen left singular vector associated with  $\sigma_i$ . Specifically, for the  $c_i$  multiple  $\sigma_i$ , the orthonormal basis of the corresponding left singular subspace can be chosen so that  $b$  has a nonzero orthogonal projection on just one unit length left singular vector  $u_i$  in the singular subspace and no components in the remaining  $c_i - 1$  ones. Precisely, let the columns of  $F_i$  form an orthonormal basis of the left singular subspace associated with  $\sigma_i$ , each of which satisfies (1.6). Then we take

$$(7.1) \quad u_i = \frac{F_i F_i^T b}{\|F_i^T b\|},$$

where  $F_i F_i^T$  is the orthogonal projector onto the left singular subspace with  $\sigma_i$ , and define the corresponding unit length right singular vector by  $v_i = A^T u_i / \sigma_i$ . We select the other  $c_i - 1$  orthonormal left singular vectors which are orthogonal to  $u_i$  and, together with  $u_i$ , form the left singular subspace associated with  $\sigma_i$ , and define the corresponding unit length right singular vectors in the same way as  $v_i$ , which and  $v_i$  form an orthonormal basis of the unique right singular subspace with  $\sigma_i$ . After such treatment, we get the desired SVD of  $A$ . We stress that  $u_i$  defined above is unique since the orthogonal projection of  $b$  onto the left singular subspace with  $\sigma_i$  is unique and equal to  $F_i F_i^T b$  for a given orthonormal  $F_i$ .

Now we need to prove that  $u_i$  satisfies the discrete Picard condition (1.6) essentially. To see this, by the Cauchy–Schwarz inequality, (7.1) and the assumption that each column of  $F_i$  satisfies the discrete Picard condition (1.6), we get

$$(7.2) \quad |u_i^T \hat{b}| = \frac{|b^T F_i F_i^T \hat{b}|}{\|F_i^T \hat{b}\|} \leq \|F_i^T \hat{b}\| = \sqrt{c_i} \sigma_i^{1+\beta}, \quad i = 1, 2, \dots, s.$$

Therefore, the Fourier coefficients  $|u_i^T \hat{b}|$ , on average, decay faster than the singular values  $\sigma_i$ ,  $i = 1, 2, \dots, s$ . This is exactly what the discrete Picard condition means; see the description before (1.6). Recall that (1.6) is a simplified model of this condition. Based on the estimate (7.2), we recover (1.6) by simply resetting (7.2) as

$$(7.3) \quad |u_i^T \hat{b}| = \sigma_i^{1+\beta}, \quad i = 1, 2, \dots, s.$$

With help of the SVD of  $A$  described above, it is crucial to observe that  $x_k^{tsvd}$  in (1.8) is now the sum consisting of the first  $k$  *distinct* dominant SVD components of  $A$ . Furthermore, for (1.1) and such reformulation of (1.8), the matrix  $A$  in them can be equivalently replaced by the new  $m \times n$  matrix

$$(7.4) \quad A' = U \Sigma' V^T,$$

where  $\Sigma' = \text{diag}(\sigma_1, \sigma_2, \dots, \sigma_s, \mathbf{0})$ ,  $U_s = (u_1, u_2, \dots, u_s)$  and  $V_s = (v_1, v_2, \dots, v_s)$  are the first  $s$  columns of  $U$  and  $V$ , respectively, the last  $n - s$  columns of  $U$  are the other left singular vectors of  $A$  that are orthogonal to  $b$  by the construction stated above, and the last  $n - s$  columns of  $V$  are the other corresponding right singular vectors of  $A$ . Obviously, for the new SVD of  $A$  defined above,  $A'$  is of rank  $s$  with the  $s$  simple nonzero singular values  $\sigma_1, \sigma_2, \dots, \sigma_s$ , its left and right singular vector matrices  $U$  and  $V$  are the corresponding ones of  $A$  with proper column exchanges, respectively. We have  $x_{true} = A^\dagger \hat{b} = (A')^\dagger \hat{b}$  and the TSVD regularized solutions  $x_k^{tsvd} = (A'_k)^\dagger \hat{b}$ , where  $A'_k$  is the best rank  $k$  approximation to  $A'$  with respect to the 2-norm. In addition,

we comment that from the discrete Picard condition

$$\|A^\dagger \hat{b}\| = \|(A')^\dagger \hat{b}\| = \left( \sum_{k=1}^s \frac{|u_k^T \hat{b}|^2}{\sigma_k^2} \right)^{1/2} \leq C,$$

independently of  $n$  and  $s$ , we can obtain (7.3) directly in the same way as done in the introduction for (1.6).

Another fundamental change is that the  $k$ -dimensional dominant right singular space of  $A$  now becomes that of  $A'$ , i.e.,  $\mathcal{V}_k = \text{span}\{V_k\}$  with  $V_k = (v_1, v_2, \dots, v_k)$  associated with the first  $k$  large singular values of  $A'$ . It is the subspace of concern in the case that  $A$  has multiple singular values. We will also denote  $U_k = (u_1, u_2, \dots, u_k)$  and  $\mathcal{U}_k = \text{span}\{U_k\}$ . As for Krylov subspaces, by the SVD of  $A$  and that of  $A'$ , expanding  $b$  as  $b = \sum_{j=1}^s \xi_j u_j + (I - U_s U_s^T)b$ , we easily justify

$$(7.5) \quad \mathcal{K}_k(A^T A, A^T b) = \mathcal{K}_k((A')^T A', (A')^T b)$$

and

$$(7.6) \quad \mathcal{K}_k(AA^T, b) = \mathcal{K}_k(A'(A')^T, b)$$

by noting that

$$(7.7) \quad (A^T A)^i A^T b = ((A')^T A')^i (A')^T b = \sum_{j=1}^s \xi_j \sigma_j^{2i+1} v_j$$

for any integer  $i \geq 0$  and

$$(7.8) \quad (AA^T)^i b = (A'(A')^T)^i b = \sum_{j=1}^s \xi_j \sigma_j^{2i} u_j$$

for any integer  $i \geq 1$ . Thus, for the given  $b$ , Lanczos bidiagonalization works on  $A$  exactly as if it does on  $A'$ . That is, (2.1)–(2.4) generated by Algorithm 1 hold when  $A$  is replaced by  $A'$ , and the  $k$  Ritz values  $\theta_i^{(k)}$  approximate  $k$  nonzero singular values of  $A'$ . Moreover, (7.7) and (7.8) indicate

$$\mathcal{K}_{s+1}((A')^T A', (A')^T b) = \mathcal{K}_s((A')^T A', (A')^T b), \quad \mathcal{K}_{s+2}(A'(A')^T, b) = \mathcal{K}_{s+1}(A'(A')^T, b).$$

As a result, since  $(A')^T b$  has nonzero components in all the eigenvectors  $v_1, v_2, \dots, v_s$  of  $(A')^T A'$  associated with its nonzero distinct eigenvalues  $\sigma_1^2, \sigma_2^2, \dots, \sigma_s^2$ , Lanczos bidiagonalization cannot break down until step  $s+1$ , and the singular values  $\theta_i^{(s)}$  of  $B_s$  are exactly the singular values  $\sigma_1, \sigma_2, \dots, \sigma_s$  of  $A'$ . At step  $s$ , Lanczos bidiagonalization on  $A$  generates the  $(s+1) \times s$  lower bidiagonal matrix

$$(7.9) \quad P_{s+1}^T A Q_s = P_{s+1}^T A' Q_s = B_s$$

and

$$(7.10) \quad \mathcal{V}_s = \text{span}\{Q_s\}, \quad \mathcal{U}_s \subset \text{span}\{P_{s+1}\}.$$

Having done the above, what we need is to estimate how  $\mathcal{K}_k(A^T A, A^T b) = \mathcal{K}_k((A')^T A', (A')^T b)$  approximates or captures the  $k$ -dimensional dominant right subspaces  $\mathcal{V}_k$ ,  $k = 1, 2, \dots, s-1$ . This is a crucial step and the starting point of all the

later analysis. In what follows let us show how to adapt the beginning part of the proof of Theorem 3.1 to the case that  $A$  has multiple singular values.

Observe the Krylov subspace  $\mathcal{K}_k((\Sigma')^2, \Sigma' U^T b) = \text{span}\{\hat{D}\hat{T}_k\}$  with

$$\hat{D} = \text{diag}(\sigma_1 u_1^T b, \dots, \sigma_s u_s^T b, \mathbf{0}) = \begin{pmatrix} D & \\ & \mathbf{0} \end{pmatrix} \in \mathbb{R}^{n \times n}$$

and

$$\hat{T}_k = \begin{pmatrix} 1 & \sigma_1^2 & \dots & \sigma_1^{2k-2} \\ 1 & \sigma_2^2 & \dots & \sigma_2^{2k-2} \\ \vdots & \vdots & & \vdots \\ 1 & \sigma_s^2 & \dots & \sigma_s^{2k-2} \\ 0 & 0 & \dots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \dots & 0 \end{pmatrix} = \begin{pmatrix} T_k \\ \mathbf{0} \end{pmatrix} \in \mathbb{R}^{n \times k}.$$

Partition the diagonal matrix  $D$  and the matrix  $T_k$  into the forms

$$D = \begin{pmatrix} D_1 & 0 \\ 0 & D_2 \end{pmatrix} \in \mathbb{R}^{s \times s}, \quad T_k = \begin{pmatrix} T_{k1} \\ T_{k2} \end{pmatrix} \in \mathbb{R}^{s \times k},$$

where  $D_1, T_{k1} \in \mathbb{R}^{k \times k}$  and  $D_2 = \text{diag}(u_{k+1}^T b, \dots, u_s^T b)$ . Since  $T_{k1}$  is a Vandermonde matrix with  $\sigma_j$  distinct for  $j = 1, 2, \dots, k$ , it is nonsingular. Therefore, from

$$\mathcal{K}_k((A')^T A', (A')^T b) = \text{span}\{V \hat{D} \hat{T}_k\}$$

and the structures of  $\hat{D}$  and  $\hat{T}_k$ , we obtain

$$\mathcal{K}_k((A')^T A', (A')^T b) = \text{span}\{V_s D T_k\} = \text{span}\left\{V_s \begin{pmatrix} D_1 T_{k1} \\ D_2 T_{k2} \end{pmatrix}\right\} = \text{span}\left\{V_s \begin{pmatrix} I \\ \Delta_k \end{pmatrix}\right\},$$

with

$$\Delta_k = D_2 T_{k2} T_{k1}^{-1} D_1^{-1},$$

meaning that  $\mathcal{K}_k((A')^T A', (A')^T b)$  is orthogonal to the last  $n - s$  columns of  $V$ .

Write

$$(7.11) \quad V_s = (V_k, V_k^\perp), \quad V = (V_s, \hat{V}_s),$$

and define

$$Z_k = V_s \begin{pmatrix} I \\ \Delta_k \end{pmatrix} = V_k + V_k^\perp \Delta_k.$$

Then  $Z_k^T Z_k = I + \Delta_k^T \Delta_k$ , the columns of  $\hat{Z}_k = Z_k (Z_k^T Z_k)^{-\frac{1}{2}}$  form an orthonormal basis of  $\mathcal{K}_k((A')^T A', (A')^T b)$ , and we get the orthogonal direct sum decomposition

$$\hat{Z}_k = (V_k + V_k^\perp \Delta_k) (I + \Delta_k^T \Delta_k)^{-\frac{1}{2}}.$$

Denote  $\mathcal{V}_k^R = \mathcal{K}_k((A')^T A', (A')^T b)$ . For  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$ , based on the above, we get (3.3) by replacing  $V_k^\perp$  in (3.14) by  $(V_k^\perp, \hat{V}_s)$  defined as (7.11) and noting that  $\hat{Z}_k$

is orthogonal to  $\hat{V}_s$ . Then it is direct to derive the same bounds for  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  as those established previously in completely the same way.

As for the extension of Theorem 3.4, by definition and (7.11), we need to replace  $V_k^\perp$  in (3.47) by  $(V_k^\perp, \hat{V}_s)$  defined as (7.11). The unit-length  $\tilde{q}_k \in \mathcal{V}_k^R$  is now a vector that has the smallest acute angle with  $\text{span}\{(V_k^\perp, \hat{V}_s)\}$ , and we modify (3.48) as

$$\tilde{q}_k = \hat{V}_s \hat{V}_s^T \tilde{q}_k + V_k^\perp (V_k^\perp)^T \tilde{q}_k + V_k V_k^T \tilde{q}_k.$$

Recall that the columns of  $\hat{V}_s$  are the right singular vectors of  $A'$  corresponding to zero singular values. It disappears when forming the Rayleigh quotient of  $(A')^T A'$  with respect to  $\tilde{q}_k$ . The proof of Theorem 3.4 then carries over to  $A'$ , and the results hold for the case that  $A$  has multiple singular values.

Another fundamental change is that, when speaking of a rank  $k$  approximation, we now mean that for  $A'$ . Note that the best rank  $k$  approximation  $A'_k$  to  $A'$  is  $A'_k = U_k \Sigma'_k V_k^T$ ,  $k = 1, 2, \dots, s$ , where  $U_k$  and  $V_k$  are defined as before, and  $\Sigma'_k = \text{diag}(\sigma_1, \sigma_2, \dots, \sigma_k)$ . The  $k$ -step Lanczos bidiagonalization process on  $A$  now generates rank  $k$  approximations  $P_{k+1} B_k Q_k^T$  in LSQR and  $P_k \bar{B}_{k-1} Q_k$  in CGME to  $A'$  and the rank  $k$  approximation  $Q_{k+1} Q_{k+1}^T (A')^T A' Q_k Q_k^T$  in LSMR to  $(A')^T A'$ , where  $P_{k+1}$  and  $Q_k$  are the first  $k+1$  and  $k$  columns of  $P_{s+1}$  and  $Q_s$  in (7.9). We then need to estimate the approximation accuracy of these rank  $k$  approximations and compare them with that of the best rank  $k$  approximations  $A'_k$  and  $(A'_k)^T A'_k$ , respectively. Meanwhile, for each of these three rank  $k$  approximation matrices, we need to analyze how its  $k$  nonzero singular values approximate  $k$  singular values of  $A'$  or  $(A')^T A'$ .

For the rank  $k$  approximation  $P_{k+1} B_k Q_k^T$  to  $A'$  in LSQR, similar to (4.1), we define

$$\gamma'_k = \|A' - P_{k+1} B_k Q_k^T\|, \quad k = 1, 2, \dots, s-1.$$

Then, without any changes but the replacement of the index  $n$  by  $s$ , all the results in Section 4 and (5.17) in Theorem 5.1 carry over to the multiple singular value case.

The final important note is how to extend the results presented Section 5.1–5.3 to the multiple singular value case. We have to derive the three key relations similar to (5.5), (5.6) and (5.7), where the fact that Lanczos bidiagonalization can be run to  $n$  steps without breakdown is exploited. In the case that  $A$  has multiple singular values, since Lanczos diagonalization on  $A$  must break down at step  $s+1$ , there are no  $P_{n+1}$  and  $Q_n$  as in (5.5). To this end, from (7.9) we augment  $P_{s+1}$  and  $Q_s$  to the  $m \times m$  and  $n \times n$  orthogonal matrices  $P = (P_{s+1}, \hat{P})$  and  $Q = (Q_s, \hat{Q})$ , respectively, from which and (7.9) we obtain

$$P^T A Q = P^T A' Q = \begin{pmatrix} B_s & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}.$$

Having this relation, like (5.5) and (5.6), we get

$$\gamma'_k = \|A' - P_{k+1} B_k Q_k^T\| = \|P^T (A' - P_{k+1} B_k Q_k^T) Q\| = \|G_k\|,$$

where  $G_k$  is the right bottom  $(s-k+1) \times (s-k)$  matrix of  $B_s$ , similar to  $G_k$  in (5.7). Then Theorem 5.1 extends naturally to the multiple singular value case without any change but the replacement of the index  $n$  by  $s$ , and all the other results and analysis in Section 5.1–5.3 carry over to this case as well. The results in Section 6 hold without any change whenever  $A$ ,  $A_k$  and the index  $n$  are replaced by  $A'$ ,  $A'_k$  and  $s$ , respectively.

In summary, based on the above reformulations, changes and preliminary work, except Section 5.4, we have extended all the results and analysis in Sections 2–6 to the case that  $A$  has multiple singular values, just as we have done for the simple singular value case. In the analysis, derivation and results, the index  $n$  is often replaced by  $s$  whenever needed, and when this is necessary is clear from the context related.

**8. Numerical experiments.** For a number of problems from Hansen’s regularization toolbox [54], Huang and Jia [64] have numerically justified the full regularization of LSQR for severely and moderately ill-posed problems and its partial regularization for mildly ill-posed problems, where each  $A$  is  $1,024 \times 1,024$ . In this section, we report numerical experiments to confirm our theory and illustrate the full or partial regularization of LSQR in much more detail. For the first two kinds of problems, we demonstrate that  $\gamma_k$ ,  $\alpha_{k+1}$  and  $\beta_{k+2}$  decay as fast as  $\sigma_{k+1}$ . We compare LSQR and the hybrid LSQR with the TSVD method applied to projected problems after semi-convergence. In the experiments, we use the L-curve criterion, the function `lcorner` in [54], to determine an actually optimal regularization parameter. For each of severely and moderately ill-posed problems, we show that the regularized solution obtained by LSQR at semi-convergence is at least as accurate as the best TSVD regularized solution, indicating that LSQR has the full regularization. In the meantime, we show that the regularized solution obtained by LSQR at semi-convergence is considerably less accurate than that by the hybrid LSQR for mildly ill-posed problems, demonstrating that LSQR has only the partial regularization. As a byproduct, we compare LSQR with GMRES and RRGMR and illustrate that the latter ones have no regularizing effects for general nonsymmetric ill-posed problems.

We choose several ill-posed problems from Hansen’s regularization toolbox [54], which include the severely ill-posed problems `shaw`, `wing`, `ilaplace`, the moderately ill-posed problems `heat`, `phillips`, and the mildly ill-posed problem `deriv2`. All the codes are from [54], and the problems arise from discretizations of (1.2). We remind that, as far as solving (1.1) is concerned, our primary goal consists in justifying the regularizing effects of iterative solvers for (1.1), which are *unaffected by the size* of (1.1) and only depends on the degree of ill-posedness, the noise level  $\|e\|$  and the actual discrete Picard condition, provided that the condition number of (1.1), measured by the ratio between the largest and smallest singular values of each  $A$ , is large enough. Therefore, for this purpose, as extensively done in the literature (see, e.g., [53, 56] and the references therein as well as many other papers), it is enough to report the results on small and/or medium sized discrete ill-posed problems since the condition numbers of these  $A$  are already huge or large, which, in finite precision arithmetic, are roughly  $10^{16}$ ,  $10^8$  and  $10^6$  for severely, moderately and mildly ill-posed problems with  $n = 256$ , respectively. Indeed, for  $n$  large, say, 10,000 or more, we have observed that LSQR and the hybrid LSQR have the same behavior as for small  $n$ , e.g.,  $n = 256$  used in this paper. Also, an important reason is that such choice enables us to fully justify the regularization effects of LSQR by comparing it with the TSVD method, which suits only for small and/or medium sized problems because of its computational complexity for  $n$  large. For each example, we generate a  $256 \times 256$  matrix  $A$ , the true solution  $x_{true}$  and noise-free right-hand side  $\hat{b}$ . In order to simulate the noisy data, we generate white noise vectors  $e$  such that the relative noise levels  $\varepsilon = \frac{\|e\|}{\|\hat{b}\|} = 10^{-2}, 10^{-3}, 10^{-4}$ , respectively. We mention that, to better illustrate the behavior of the hybrid LSQR, we, in the concluding section, will report some important observations on `phillips` and `deriv2` of  $n = 1,024$  and  $10,240$ , whose condition numbers are as large as  $1.7 \times 10^{15}$  and  $1.3 \times 10^8$  for  $n = 10,240$ , respectively. To simulate exact arithmetic, LSQR



uses full reorthogonalization in Lanczos bidiagonalization. All the computations are carried out in Matlab 7.8 with the machine precision  $\epsilon_{\text{mach}} = 2.22 \times 10^{-16}$  under the Microsoft Windows 7 64-bit system.

**8.1. The accuracy of rank  $k$  approximations. Example 1.** This problem **shaw** arises from one-dimensional image restoration and is obtained by discretizing (1.2) with  $[-\frac{\pi}{2}, \frac{\pi}{2}]$  as the domains of  $s$  and  $t$ , where

$$k(s, t) = (\cos(s) + \cos(t))^2 \left( \frac{\sin(u)}{u} \right)^2, \quad u = \pi(\sin(s) + \sin(t)),$$

$$x(t) = 2 \exp(-6(t - 0.8)^2) + \exp(-2(t + 0.5)^2).$$

**Example 2.** This problem **wing** has a discontinuous solution and is obtained by discretizing (1.2) with  $[0, 1]$  as the domains of  $s$  and  $t$ , where

$$k(s, t) = t \exp(-st^2), \quad g(s) = \frac{\exp(-\frac{1}{9}s) - \exp(-\frac{4}{9}s)}{2s},$$

$$x(t) = \begin{cases} 1, & \frac{1}{3} < t < \frac{2}{3}; \\ 0, & \text{elsewhere.} \end{cases}$$

The problems **shaw** and **wing** are severely ill-posed with the singular values  $\sigma_k = \mathcal{O}(e^{-4k})$  for **shaw** and  $\sigma_k = \mathcal{O}(e^{-9k})$  for **wing**, respectively.

In Figure 1, we display the decay curves of the  $\gamma_k$  for **shaw** with  $\varepsilon = 10^{-2}, 10^{-3}$  and for **wing** with  $\varepsilon = 10^{-3}, 10^{-4}$ , respectively. We observe that the three curves with different  $\varepsilon$  are almost unchanged. This is in accordance with our Remark 4.1, where it is stated that the decay rate of  $\gamma_k$  is little affected by noise levels for severely ill-posed problems, since  $\gamma_k$  primarily depends on the decay rate of  $\sigma_{k+1}$  and different noise levels only affect the value of  $k_0$  other than the decay rate of  $\gamma_k$ . In addition, we have observed that  $\gamma_k$  and  $\sigma_{k+1}$  decay until they level off at  $\epsilon_{\text{mach}}$  due to round-off errors. Most importantly, the results have clearly confirmed the theory that  $\gamma_k$  decreases as fast as  $\sigma_{k+1}$ , and we have  $\gamma_k \approx \sigma_{k+1}$ , whose decay curves are almost indistinguishable.

In Figure 2, we plot the relative errors  $\|x^{(k)} - x_{\text{true}}\| / \|x_{\text{true}}\|$  with different  $\varepsilon$  for these two problems. As we have seen, LSQR exhibits clear semi-convergence. Moreover, for a smaller  $\varepsilon$ , we get a more accurate regularized solution at cost of more iterations, as  $k_0$  is bigger from (1.6) and (1.7).

**Example 3.** This problem **heat** is moderately ill-posed, arises from the inverse heat equation, and is obtained by discretizing (1.2) with  $[0, 1]$  as integration interval, where the kernel  $k(s, t) = k(s - t)$  with

$$k(t) = \frac{t^{-3/2}}{2\sqrt{\pi}} \exp\left(-\frac{1}{4t}\right).$$

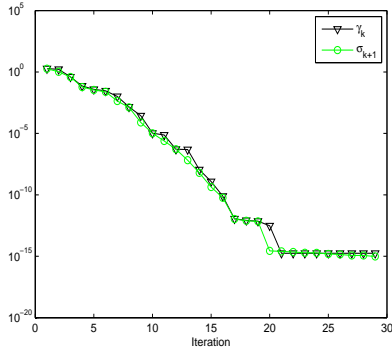
**Example 4.** This is the **phillips** famous problem, a moderately ill-posed one. It is obtained by discretizing (1.2) with  $[-6, 6]$  as the domains of  $s$  and  $t$ , where

$$k(s, t) = \begin{cases} 1 + \cos\left(\frac{\pi(s-t)}{3}\right), & |s - t| < 3, \\ 0, & |s - t| \geq 3, \end{cases}$$

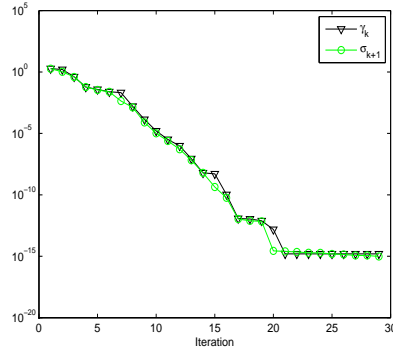
$$g(s) = (6 - |s|) \left(1 + \frac{1}{2} \cos\left(\frac{\pi s}{3}\right)\right) + \frac{9}{2\pi} \sin\left(\frac{\pi|s|}{3}\right),$$

$$x(t) = \begin{cases} 1 + \cos\left(\frac{\pi t}{3}\right), & |t| < 3, \\ 0, & |t| \geq 3. \end{cases}$$

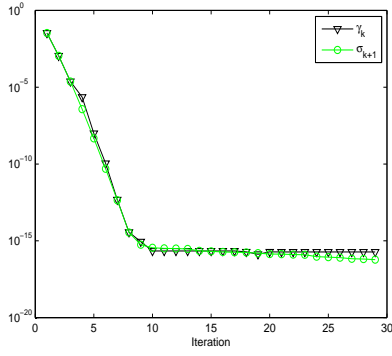




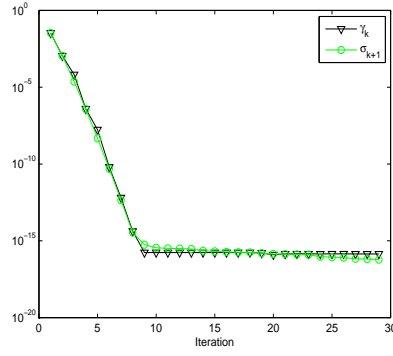
(a)



(b)

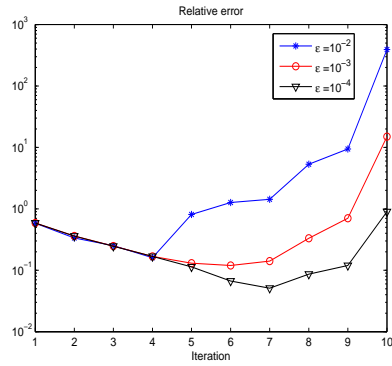


(c)

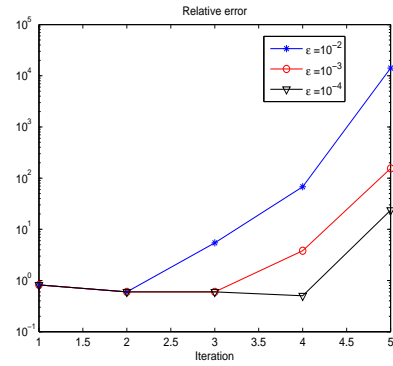


(d)

FIG. 1. (a)-(b): Decay curves of the sequences  $\gamma_k$  and  $\sigma_{k+1}$  for *shaw* with  $\varepsilon = 10^{-2}$  (left) and  $\varepsilon = 10^{-3}$  (right); (c)-(d): Decay curves of the sequences  $\gamma_k$  and  $\sigma_{k+1}$  for *wing* with  $\varepsilon = 10^{-3}$  (left) and  $\varepsilon = 10^{-4}$  (right).



(a)



(b)

FIG. 2. The relative errors  $\|x^{(k)} - x_{true}\|/\|x_{true}\|$  with  $\varepsilon = 10^{-2}, 10^{-3}, 10^{-4}$  for *shaw* (left) and *wing* (right).

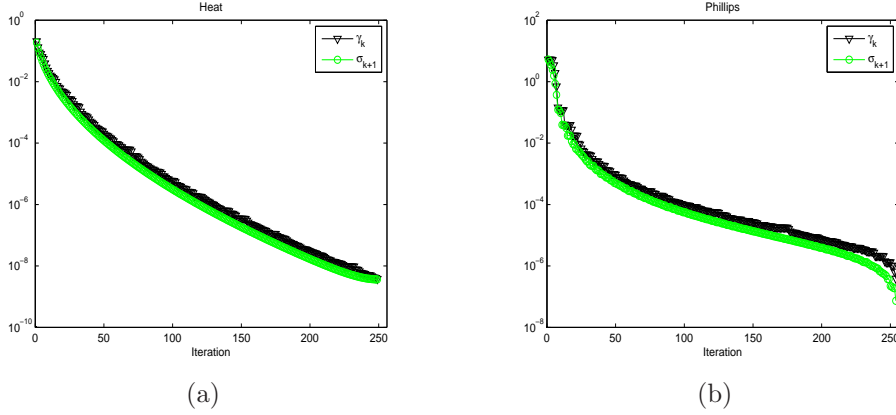


FIG. 3. (a): Decay curves of the sequences  $\gamma_k$  and  $\sigma_{k+1}$  for heat with (left) and (b): Decay curves of the sequences  $\gamma_k$  and  $\sigma_{k+1}$  for phillips with  $\varepsilon = 10^{-3}$  (right).

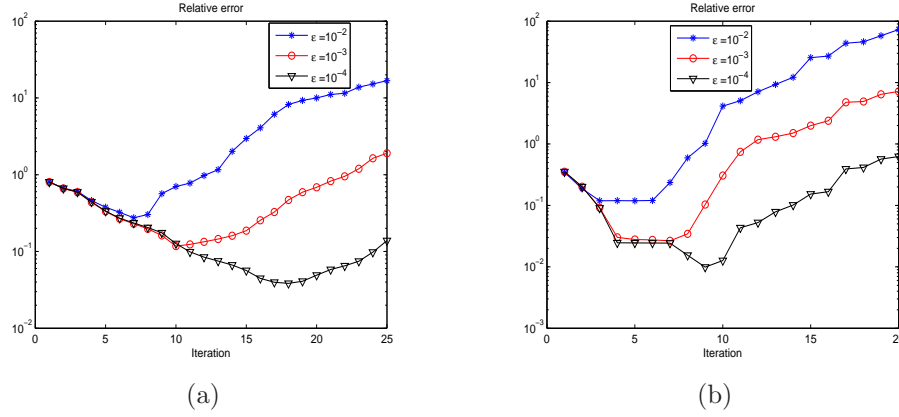


FIG. 4. The relative errors  $\|x^{(k)} - x_{true}\|/\|x_{true}\|$  with  $\varepsilon = 10^{-2}, 10^{-3}, 10^{-4}$  for heat (left) and phillips (right).

From Figure 3, we see that  $\gamma_k$  decreases almost as fast as  $\sigma_{k+1}$  for the moderately ill-posed problems heat and phillips. However, slightly different from severely ill-posed problems,  $\gamma_k$ , though excellent approximations to  $\sigma_{k+1}$ , may not be so very accurate. This is expected, as the constants  $\eta_k$  in (4.4) are generally bigger than those in (4.3) for severely ill-posed problems. Also, different from Figure 1, we observe from Figure 3 that  $\gamma_k$  deviates more from  $\sigma_{k+1}$  with  $k$  increasing, especially for the problem phillips. This confirms Remarks 4.1–4.3 on moderately ill-posed problems.

In Figure 4, we depict the relative errors of  $x^{(k)}$ , and from them we observe analogous phenomena to those for severely ill-posed problems. The only distinction is that LSQR now needs more iterations, i.e., a bigger  $k_0$  is needed for moderately ill-posed problems with the same  $\varepsilon$ , as is seen from (1.6) and (1.7).

**Example 5.** The mildly ill-posed problem deriv2 is obtained by discretizing (1.2) with  $[0, 1]$  as the domains of  $s$  and  $t$ , where the kernel  $k(s, t)$  is the Green's function for the second derivative:

$$k(s, t) = \begin{cases} s(t-1), & s < t; \\ t(s-1), & s \geq t, \end{cases}$$

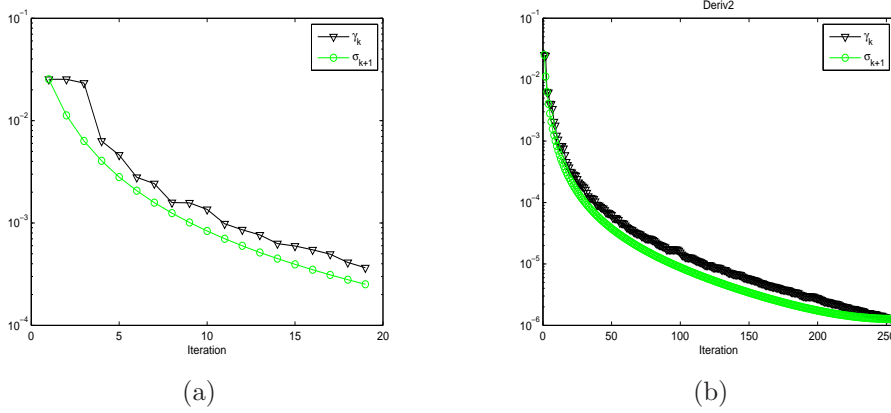


FIG. 5. (a)-(b): Decay curves of the partial and complete sequences  $\gamma_k$  and  $\sigma_{k+1}$  for deriv2 with  $\varepsilon = 10^{-3}$

and the solution  $x(t)$  and the right-hand side  $g(s)$  are given by

$$x(t) = \begin{cases} t, & t < \frac{1}{2}; \\ 1-t, & t \geq \frac{1}{2}, \end{cases} \quad g(s) = \begin{cases} (4s^3 - 3s)/24, & s < \frac{1}{2}; \\ (-4s^3 + 12s^2 - 9s + 1)/24, & s \geq \frac{1}{2}. \end{cases}$$

Figure 5 (a)-(b) display the decay curves of the partial and complete sequences  $\gamma_k$  and  $\sigma_{k+1}$ , respectively. We see that, different from severely and moderately ill-posed problems,  $\gamma_k$  does not decay so fast as  $\sigma_{k+1}$  and deviates from  $\sigma_{k+1}$  significantly. Recall that Theorem 4.1 holds for mildly ill-posed problems, where  $\eta_k$  defined by (4.4) is considerably bigger than one. These observations justify our theory and confirm that the rank  $k$  approximations to  $A$  generated by Lanczos bidiagonalization are not as accurate as those for severely and moderately problems.

**8.2. A comparison of LSQR and the hybrid LSQR.** For the severely ill-posed shaw, wing and the moderately ill-posed heat, phillips, we compare the regularizing effects of LSQR and the hybrid LSQR with the TSVD method applied to the projected problems after semi-convergence, and demonstrate that they compute the same best possible regularized solution for each problem and LSQR thus has the full regularization. For the mildly ill-posed problem deriv2, we show that LSQR has only the partial regularization and the hybrid LSQR can compute a best possible regularized solution.

In the sequel, we report the results only for the noise level  $\varepsilon = 10^{-3}$ . Results for the other two  $\varepsilon$  are analogous and thus omitted unless stated otherwise.

We first have a close look at the severely and moderately ill-posed problems. Figure 6 (a)-(b) and Figure 7 (a)-(b) plot the relative errors of regularized solutions obtained by the two methods for shaw, wing and heat, phillips. Clearly, we see that for each problem the relative errors reach the same minimum level. After semi-convergence of LSQR, the TSVD method applied to projected problems simply stabilizes the regularized solutions with the minimum error and does not improve them. This means that LSQR has already found best possible regularized solutions at semi-convergence and has the full regularization, and regularization applied to projected problems does not help and is unnecessary at all. In practice, we simply stop LSQR after its semi-convergence for severely and moderately ill-posed problems.

For these four problems, for test purposes we choose  $x_{reg} = \arg \min_k \|x^{(k)} - x_{true}\|$  for LSQR, which are just the iterates obtained by LSQR at semi-convergence. Figure 6 (c)-(d) and Figure 7 (c)-(d) show that the regularized solutions  $x_{reg}$  are generally excellent approximations to the true solutions  $x_{true}$ . The exception is the problem *wing* whose underlying integral equation has a discontinuous solution, which corresponds to the true solution  $x_{true}$  whose entries have big jumps in the discrete case, as depicted in Figure 6 (d). For it, the regularized solution  $x_{reg}$  deviates from  $x_{true}$  considerably and the relative error is not small. This is because all CG type methods applied to either (1.1) or  $A^T A x = A^T b$  or  $\min \|A A^T y - b\|$  with  $x = A^T y$  compute smooth regularized solutions. More insightfully, LSQR and CGLS are equivalent to implicitly solving the Tikhonov regularization problem (1.3), and their regularized solutions are of the filtered form (3.1). It is well known that the regularization term  $\lambda^2 \|x\|$  in Tikhonov regularization does not suit for discontinuous solutions. The continuous ill-posed problems with discontinuous or non-smooth solutions are from numerous important applications, including linear regression, barcode reading, gravity surveying in geophysics, image restoration and some others [1, 56, 89]. For them, a better alternative is use the 1-norm  $\lambda^2 \|Lx\|_1$  as the regularization term, which leads to the Total Variation Regularization [1, 27, 56, 89, 119] or Errors-in-Variables Modeling called in [116], where  $L \neq I$  is some  $p \times n$  matrix with no restriction to  $p$  and is typically taken to be the discrete approximation to the first or second derivative operator [56, Ch.8].

Now we investigate the behavior of LSQR and the hybrid LSQR for *deriv2*. Figure 8 (a) indicates that the relative errors of  $x^{(k)}$  by the hybrid LSQR reach a considerably smaller minimum level than those by LSQR, illustrating that LSQR has only the partial regularization. Precisely, we find that the semi-convergence of LSQR occurs at iteration  $k = 4$ , but the regularized solution is not acceptable. The hybrid LSQR uses a larger six dimensional Krylov subspace  $\mathcal{K}_6(A^T A, A^T b)$  to construct a more accurate regularized solution. We also choose  $x_{reg} = \arg \min_k \|x^{(k)} - x_{true}\|$  for LSQR and the hybrid LSQR, respectively. Figure 8 (b) indicates that the best regularized solution by the hybrid LSQR is a considerably better approximation to  $x_{true}$  than that by LSQR, especially in the non-smooth middle part of  $x_{true}$ .

**8.3. Decay behavior of  $\alpha_k$  and  $\beta_{k+1}$ .** For the severely ill-posed *shaw*, *wing* and the moderately ill-posed *heat*, *phillips*, we now illustrate that  $\alpha_k$  and  $\beta_{k+1}$  decay as fast as the singular values  $\sigma_k$  of  $A$ . We take the noise level  $\varepsilon = 10^{-3}$ . The results are similar for  $\varepsilon = 10^{-2}$  and  $10^{-4}$ .

Figure 9 illustrates that both  $\alpha_k$  and  $\beta_{k+1}$  decay as fast as  $\sigma_k$ , and for *shaw* and *wing* all of them decay swiftly and level off at  $\epsilon_{mach}$  due to round-off errors in finite precision arithmetic. Precisely, they reach the level of  $\epsilon_{mach}$  at  $k = 22$  and  $k = 8$  for *shaw* and *wing*, respectively. Such decay behavior has also been observed in [7, 31, 35], but no theoretical support was given. These experiments confirm Theorem 4.1 and Theorem 5.1, which have proved that  $\gamma_k$  decreases as fast as  $\sigma_{k+1}$  and that  $\alpha_k$ ,  $\beta_{k+1}$  and  $\alpha_k + \beta_{k+1}$  decay as fast as  $\sigma_k$ .

**8.4. A comparison of LSQR and the TSVD method.** We compare the performance of LSQR and the TSVD method for the severely ill-posed *shaw*, *wing* and moderately ill-posed *heat*, *phillips*. We take  $\varepsilon = 10^{-3}$ . For each problem, we compute the norms of regularized solutions, their relative errors and the residual norms obtained by the two methods. We plot the L-curves of the residual norms versus those of regularized solutions in the log-log scale.

Figures 10–11 indicate LSQR and the TSVD method behave very similarly for *shaw* and *wing*. They illustrate that, for *wing*, the norms of approximate solutions

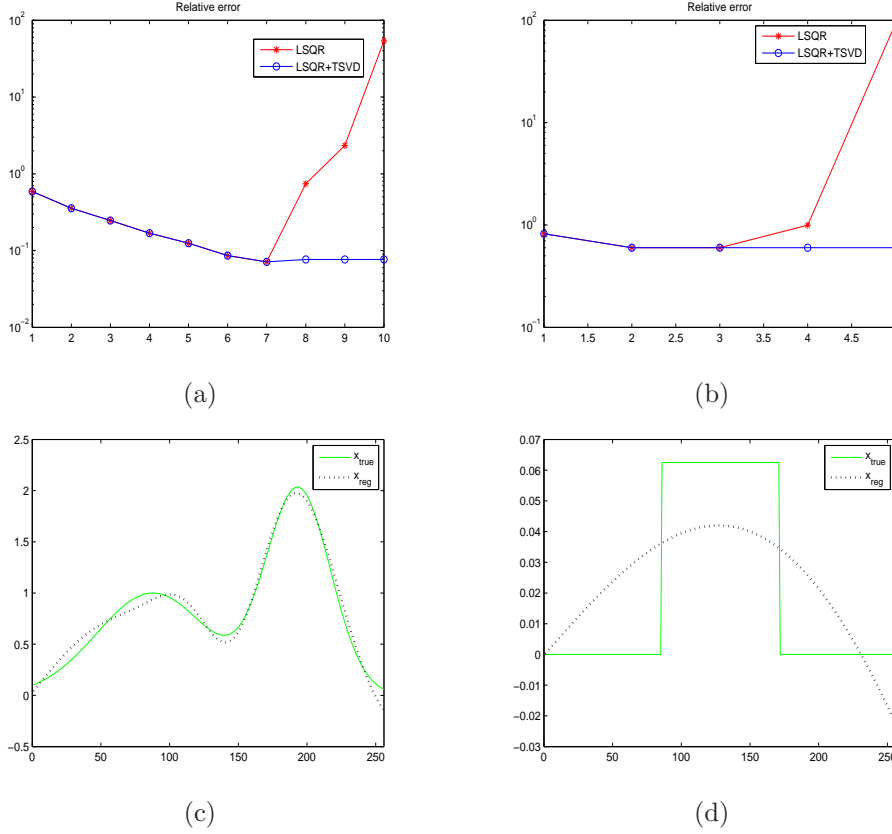
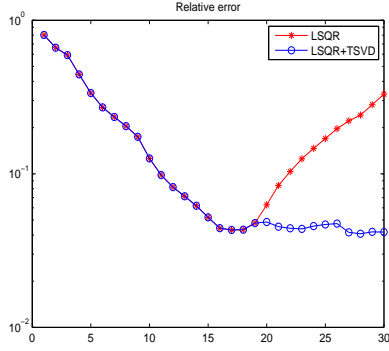


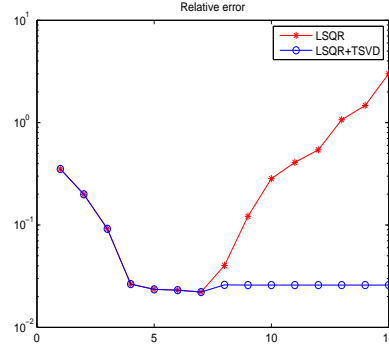
FIG. 6. (a)-(b): The relative errors  $\|x^{(k)} - x_{true}\|/\|x_{true}\|$  by LSQR and the hybrid LSQR for  $\varepsilon = 10^{-3}$ ; (c)-(d): The best regularized solutions  $x_{reg}$  by LSQR for shaw (left) and wing (right).

and the relative errors by the two methods are almost indistinguishable for the same  $k$ , and, for **shaw**, the residual norms by LSQR decreases more quickly than the ones by the TSVD method for  $k = 1, 2, 3$  and then they become almost identical starting from  $k = 4$ . The L-curves tell us that the two methods obtain the best regularized solutions when  $k_0 = 7$  and  $k_0 = 3$  for **shaw** and **wing**, respectively. The values of  $k_0$  determined by the L-curves are exactly the ones at which semi-convergence occurs, as indicated by (b) and (c) in Figures 10–11. These results demonstrate that LSQR has the full regularization and resembles the TSVD method very much.

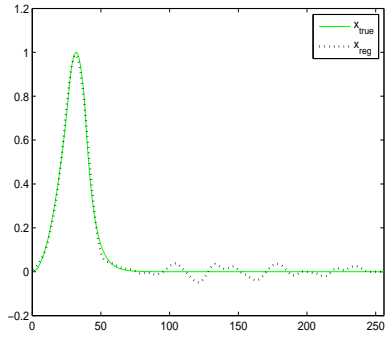
For each of **heat** and **phillips**, Figures 12–13 demonstrate that the best regularized solution obtained by LSQR is at least as accurate as, in fact, a little bit more accurate than that by the TSVD method, and the corresponding residual norms decreases and drop below at least the same level as those by the TSVD method. The residual norms by the two methods then stagnate after the best regularized solutions are found. All these confirm that LSQR has the full regularization. The fact that the best regularized solutions by LSQR can be more accurate than the best TSVD solutions is not unusual. We can explain why. Note that the true solutions  $x(t)$  to the integral equations that generate the problems **heat** and **phillips** are at least first order differentiable. It is known that, in the infinite dimensional space setting, for a linear compact operator equation  $Kx = g$ , the TSVD method and standard-form



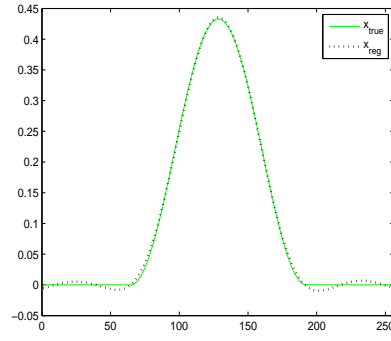
(a)



(b)

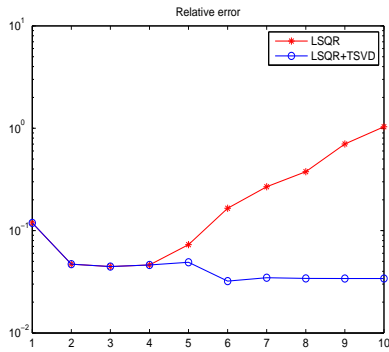


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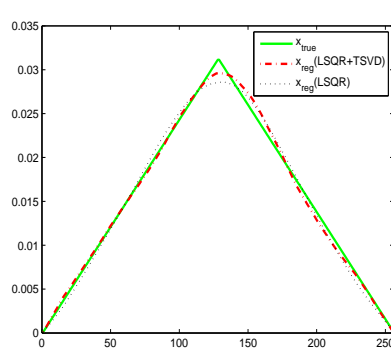


(d)

FIG. 7. (a)-(b): The relative errors  $\|x^{(k)} - x_{true}\|/\|x_{true}\|$  by LSQR and the hybrid LSQR for  $\varepsilon = 10^{-3}$ ; (c)-(d): The best possible regularized solutions  $x_{reg}$  by LSQR for heat (left) and phillips (right).



(a)



(b)

FIG. 8. (a)-(b): The relative errors  $\|x^{(k)} - x_{true}\|/\|x_{true}\|$  and the regularized solutions  $x_{reg}$  by LSQR at semi-convergence and the best possible regularized solution by the hybrid LSQR for deriv2.

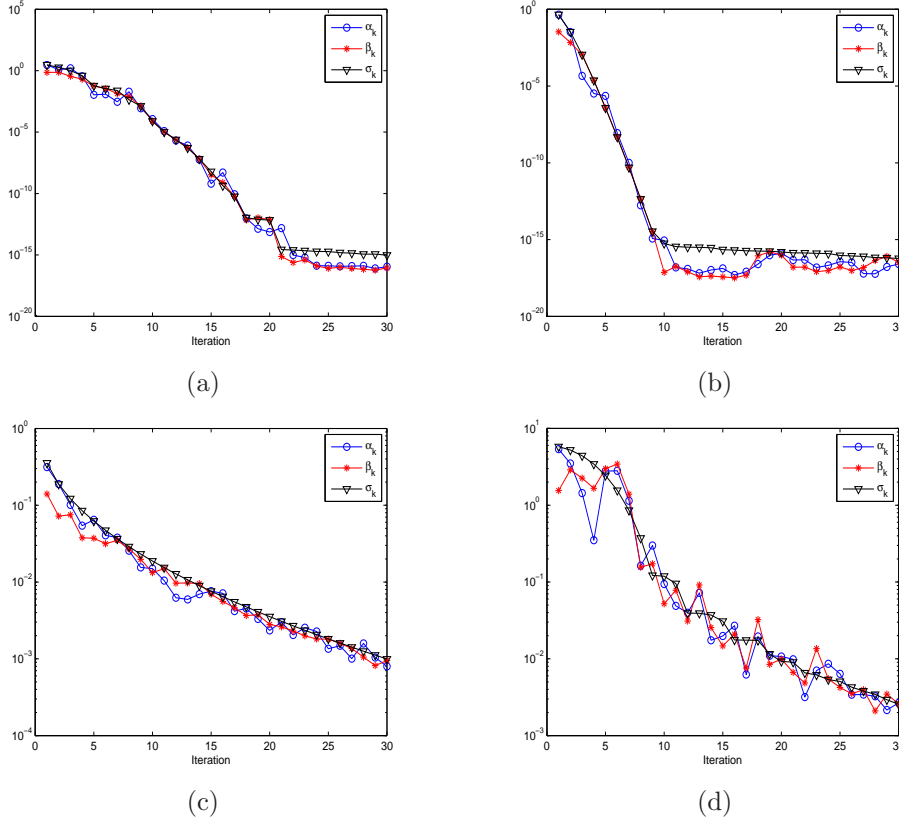


FIG. 9. (a)-(d): Decay curves of the sequences  $\alpha_k$ ,  $\beta_{k+1}$  and  $\sigma_k$  for shaw, wing, i\_laplace and heat (from top left to bottom right).

Tiknonov regularization method have been shown to be order optimal only when the true solution is continuous or first order differentiable, and they are not order optimal for stronger smoothness assumptions on the true solution. In contrast, CGLS is order optimal, and the smallest error of the iterates is of the same order as the worst-case error for the arbitrarily smooth true solution, that is, given the same noise level, the smoother the true solution is, the more accurate the best regularized solution is. In other words, for the smoother true solution, the best regularized solution by CGLS is generally more accurate than the counterpart corresponding to the continuous or first order differentiable true solution; see, e.g., [27, p.187-191] and [81, p.13,34-36,40]. Consequently, for the discrete (1.1) resulting from such kind of continuous compact linear equation, once the mathematically equivalent LSQR has the full regularization, its best regularized solution is at least as accurate as and can be more accurate than the best regularized solution by the TSVD method or the standard-form Tiknonov regularization method when the true solution of a continuous compact linear operator equation is smoother than only continuous or first order differentiable.

From the figures we observe some obvious differences between moderately and severely ill-posed problems. For heat, it is seen that the relative errors and residual norms converge considerably more quickly for the LSQR solutions than for the TSVD solutions. Figure 12 (b) tells us that LSQR only uses 12 iterations to find the best

regularized solution and the TSVD method finds the best regularized solution for  $k_0 = 21$ , while the L-curve gives 13 iterations and  $k_0 = 18$  iterations, respectively. Similar differences are observed for `phillips`, where Figure 13 (b) indicates that both LSQR and the TSVD method find the best regularized solutions at  $k_0 = 7$ , while the L-curve shows that  $k_0 = 8$  for LSQR and  $k_0 = 11$  for the TSVD method. Therefore, unlike for severely ill-posed problems, the L-curve criterion is not very reliable to determine correct  $k_0$  for moderately ill-posed problems.

We can observe more. Figure 12 shows that the TSVD solutions improve little and their residual norms decrease very slowly for the indices  $i = 4, 5, 11, 12, 18, 19, 20$ . This implies that the  $v_i$  corresponding to these indices  $i$  make very little contribution to the TSVD solutions. This is due to the fact that the Fourier coefficients  $|u_i^T \hat{b}|$  are very small relative to  $\sigma_i$  for these indices  $i$ . Note that  $\mathcal{K}_k(A^T A, A^T b)$  adapts itself in an optimal way to the specific right-hand side  $b$ , while the TSVD method uses all  $v_1, v_2, \dots, v_k$  to construct a regularized solution, independent of  $b$ . Therefore,  $\mathcal{K}_k(A^T A, A^T b)$  picks up only those SVD components making major contributions to  $x_{true}$ , such that LSQR uses possibly fewer  $k$  iterations than  $k_0$  needed by the TSVD method to capture those truly needed dominant SVD components. The fact that LSQR (CGLS) includes fewer SVD components than the TSVD solution with almost the same accuracy was first noticed by Hanke [47]. Generally, for severely and moderately ill-posed problems, we may deduce that LSQR uses possibly fewer than  $k_0$  iterations to compute a best possible regularized solution if, in practice, some of  $|u_i^T b|$ ,  $i = 1, 2, \dots, k_0$  are considerably bigger than the corresponding  $\sigma_i$  and some of them are reverse. For `phillips`, as noted by Hansen [56, p.32, 123–125], half of the SVD components satisfy  $u_i^T \hat{b} = v_i^T x_{true} = 0$  for  $i$  even, only the odd indexed  $v_1, v_3, \dots$ , make contributions to  $x_{true}$ . This is why the relative errors and residual norms of TSVD solutions do not decrease at even indices before  $x_{k_0}^{tsvd}$  is found.

**8.5. A comparison of LSQR and GMRES, RGMRES.** GMRES applied to solving (1.1) with  $A$  square computes the iterate

$$x_k^g = \|b\| W_k \bar{H}_k^\dagger e_1^{(k+1)} = W_k \bar{H}_k^\dagger W_{k+1}^T b.$$

The quantity

$$(8.1) \quad \gamma_k^g = \|A - W_{k+1} \bar{H}_k W_k^T\|$$

measures the accuracy of the rank  $k$  approximation  $W_{k+1} \bar{H}_k W_k^T$  to  $A$ , where the columns of  $W_k$  and  $W_{k+1}$  are orthonormal bases of  $\mathcal{K}_k(A, b)$  and  $\mathcal{K}_{k+1}(A, b)$ , respectively, generated by the Arnoldi process starting with  $w_1 = b/\|b\|$ , and  $\bar{H}_k = W_{k+1}^T A W_k$  is the  $(k+1) \times k$  upper Hessenberg matrix. The size of  $\gamma_k^g$  reflects the regularizing effects of GMRES for solving (1.1). We should address that, different from  $\gamma_k$  defined by (4.1) for LSQR, which has been proved to decrease monotonically as  $k$  increases (cf. (5.4)), mathematically  $\gamma_k^g$  has no monotonic property. Similar to the LSQR iterates  $x^{(k)}$  and  $\gamma_k$ , qualitatively speaking, if  $\gamma_k^g$  decays smoothly in some definitive manner, then, to some extent, GMRES has regularizing effects; if they do not decay at all or behave irregularly, then GMRES does not have regularizing effects and fails to work for (1.1). We test GMRES on the general nonsymmetric heat and the following Example 6, and compare it with LSQR.

**Example 6.** Consider the general nonsymmetric ill-posed problem `ilaplace`, which is severely ill-posed and arises from inverse Laplace transformation. It is obtained by discretizing the first kind Fredholm integral equation (1.2) with  $[0, \infty)$  the



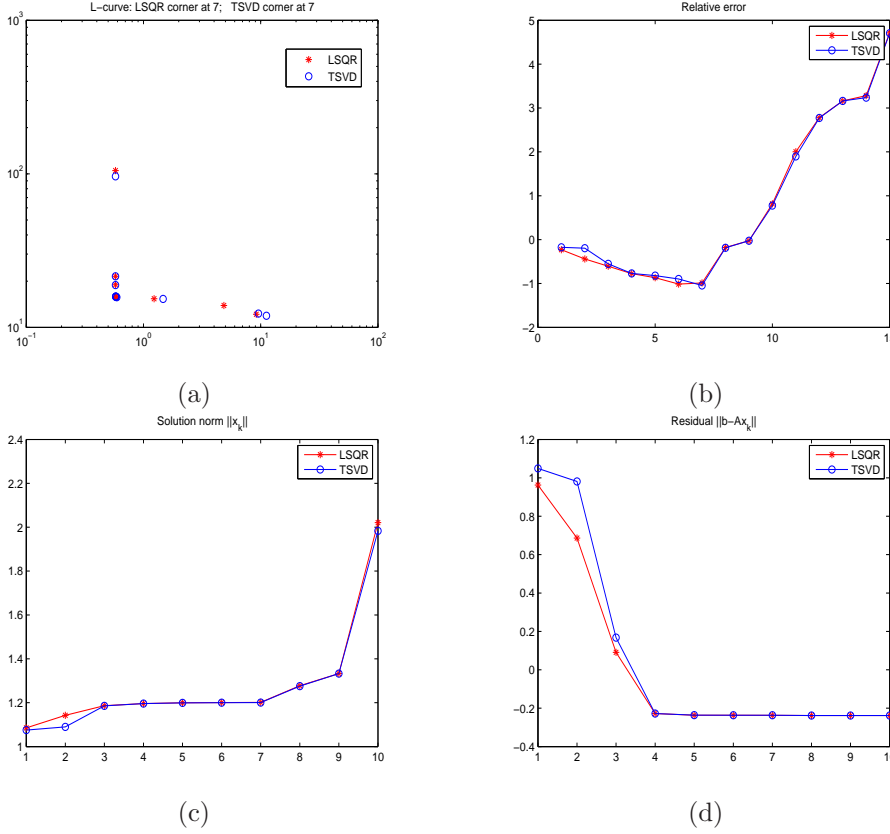


FIG. 10. Results for the severely ill-posed problem shaw.

domains of  $s$  and  $t$ . The kernel  $k(s, t)$ , the right-hand side  $g(s)$  and the solution  $x(t)$  are given by

$$k(s, t) = \exp(-st), \quad g(s) = \frac{1}{s + 1/2}, \quad x(t) = \exp(-t/2).$$

We investigate the regularizing effects of GMRES with  $\varepsilon = 10^{-3}$ . Let  $H_k = (h_{i,j}) \in \mathbb{R}^{k \times k}$  denote the upper Hessenberg matrix obtained by the  $k$ -step Arnoldi process. We observe that the  $h_{k+1,k}$  decay quickly with  $k$  increasing, generally faster than  $\sigma_k$ ; see Figure 14 (a)-(b). This phenomenon may lead to a misbelief that GMRES has general regularizing effects. However, it is not the case. In fact, a small  $h_{k+1,k}$  exactly indicates that all the eigenvalues of  $H_k$  may approximate some  $k$  eigenvalues of  $A$  well and the Arnoldi method finds an approximate  $k$ -dimensional invariant subspace or eigenspace of  $A$  [73, 104]. We also refer to [68, 69] for a detailed convergence analysis of the Arnoldi method. Unfortunately, for a general nonsymmetric matrix  $A$ , a small  $h_{k+1,k}$  does not mean that the singular values, i.e., the Ritz values, of  $\bar{H}_k$  are also good approximations to some  $k$  singular values of  $A$ . As a matter of fact, as our analysis in Section 4 and Section 5 has indicated, the accuracy of the singular values of a rank  $k$  approximation matrix, here the singular values of  $\bar{H}_k$ , as approximations to the  $k$  large singular values of  $A$  critically relies on the size of  $\gamma_k^g$  defined by (8.1) other than  $h_{k+1,k}$ . Indeed, as indicated by Figure 14 (c)-(d), though  $h_{k+1,k}$  is small, some

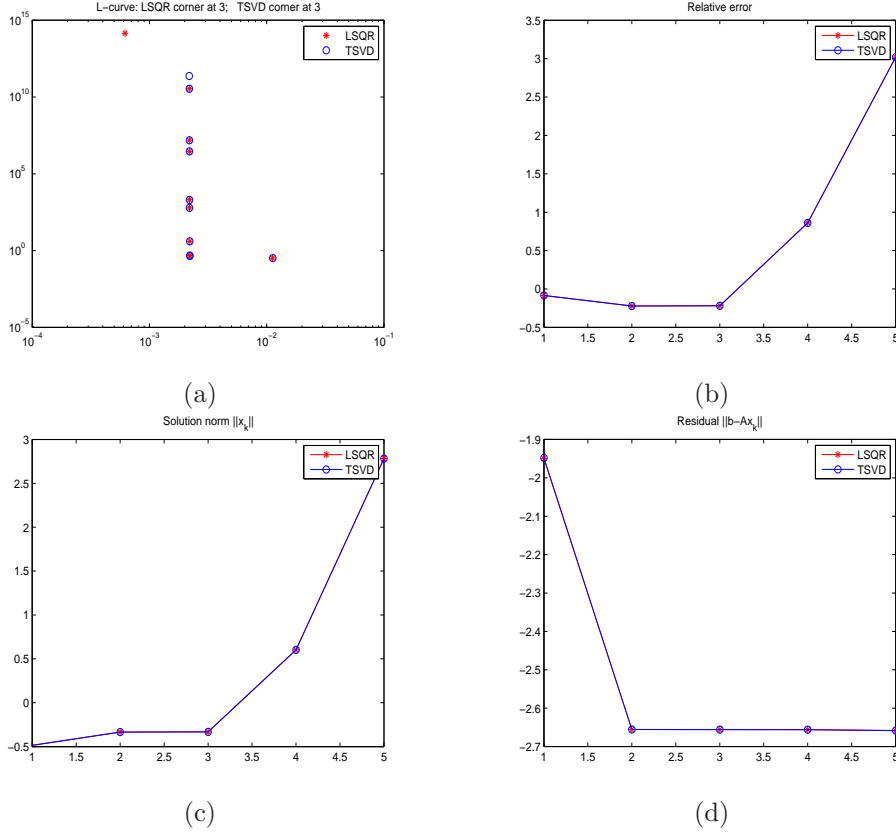


FIG. 11. Results for the severely ill-posed problem wing.

of the singular values of  $\bar{H}_k$  are very poor approximations to singular values of  $A$ , and some of those good approximations are much smaller than  $\sigma_{k+1}$  and approximate the singular values of  $A$  in disorder rather than in natural order. It is important to note that, for a general nonsymmetric or, more rigorously, non-normal  $A$ , the  $k$ -dimensional Krylov subspace  $\mathcal{K}_k(A, b)$  that underlies the Arnoldi process mixes all the left and right singular vectors of  $A$ , and the Arnoldi process generally fails to extract the dominant SVD components and cannot generate a high quality rank  $k$  approximation to  $A$ , causing that GMRES has no good regularizing effects.

Figure 15 (a)-(b) gives more justifications. We have a few important observations: For the two test problems, the quantities  $\gamma_k$  decay as fast as the  $\sigma_{k+1}$  for LSQR, while the  $\gamma_k^g$  diverge quickly from the  $\sigma_{k+1}$  for GMRES and do not exhibit any regular decreasing tendency. For `i_laplace`, the  $\gamma_k^g$  decrease very slowly until  $k = 19$ , then basically stabilize for three iterations followed, and finally start to increase from  $k = 22$  onwards. As for `heat`, the  $\gamma_k^g$  are almost constant from beginning to end. Since all the  $\gamma_k^g$  are not small, they indicate that the Arnoldi process cannot generate any reasonable and meaningful rank  $k$  approximations to  $A$  for  $k = 1, 2, \dots, 30$ . This is especially true for `heat`. Consequently, we are sure that GMRES fails and does not have regularizing effects for the two test problems.

We plot  $\|x^{(k)} - x_{true}\|/\|x_{true}\|$  by LSQR and  $\|x_k^g - x_{true}\|/\|x_{true}\|$  by GMRES in Figure 15 (c)-(d). Obviously, LSQR exhibits semi-convergence, but GMRES does not

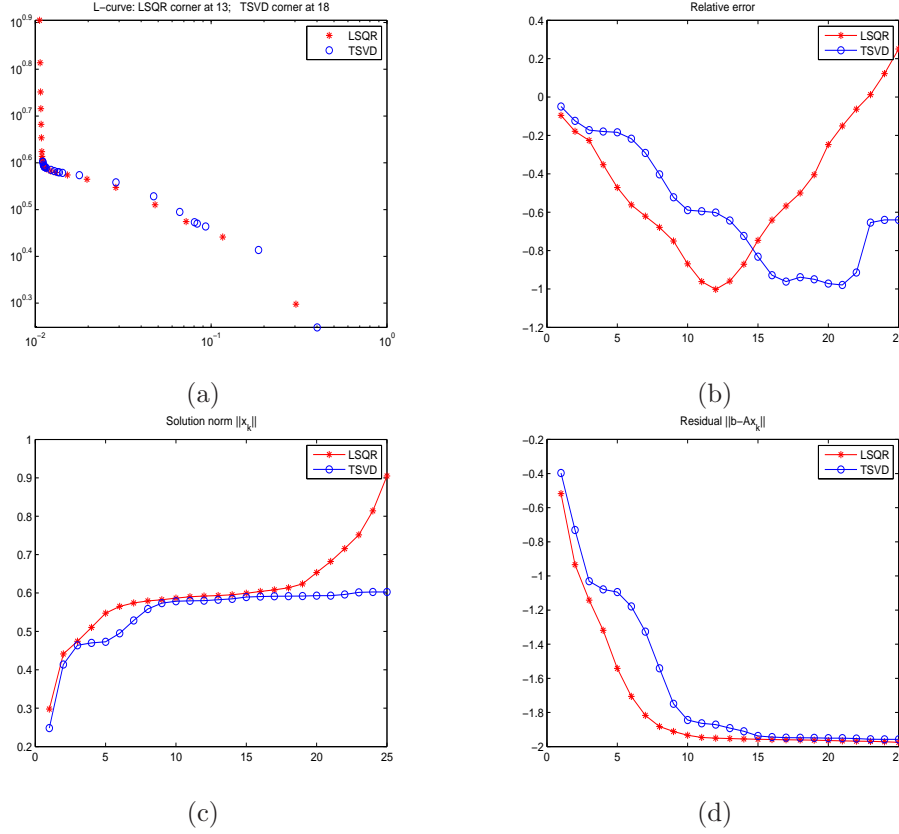


FIG. 12. Results for the moderately ill-posed problem heat.

and the relative errors obtained by it even increase from the beginning; see Figure 15 (d). This again demonstrates that GMRES cannot provide meaningful regularized solutions for these two problems. Let  $x_{reg} = \arg \min_k \|x^{(k)} - x_{true}\|$ . Figure 15 (e) and (f) show that LSQR obtains excellent regularized solutions, while GMRES fails. It is known that MR-II [29] for  $A$  symmetric and RRGMR [16] for  $A$  nonsymmetric work on the subspace  $\mathcal{K}_k(A, Ab)$ . They were originally designed to solve singular or inconsistent systems, restricted to a subspace of range of  $A$ , and compute the minimum-norm least squares solutions when the ranges of  $A$  and  $A^T$  are identical. However, for the preferred RRGMR [93], we have observed phenomena similar to those for GMRES, illustrating that RRGMR does not have regularizing effects for the test problems. From these typical experiments, we conclude that GMRES and RRGMR are susceptible to failure for general nonsymmetric ill-posed problems and they are not general-purpose regularization methods. In fact, as addressed in [56, p.126] and [67], GMRES and RRGMR may only work well when either the mixing of SVD components is weak or the Krylov basis vectors are just well suited for the ill-posed problem, as addressed in [56].

**9. Conclusions.** For the large-scale ill-posed problem (1.1), iterative solvers are the only viable approaches. Of them, LSQR and CGLS are most popularly used for general purposes, and CGME and LSMR are also choices. They have general regularizing effects and exhibit semi-convergence. However, if semi-convergence occurs before

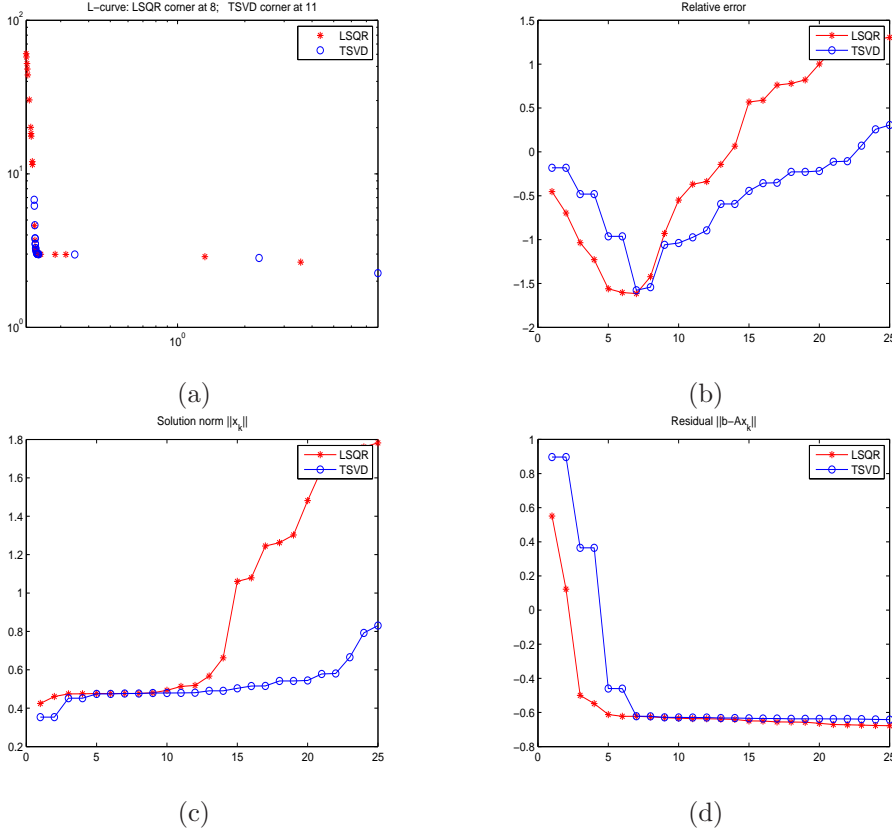


FIG. 13. Results for the moderately ill-posed problem phillips.

it capture all the needed dominant SVD components, then best possible regularized solutions are not yet found and the solvers have only the partial regularization. In this case, their hybrid variants have often been used to compute best possible regularized solutions. If semi-convergence means that they have already found best possible regularized solutions, they have the full regularization, and we simply stop them after semi-convergence.

We have considered the fundamental open question in depth: Do LSQR, CGLS, LSMR and CGME have the full or partial regularization for severely, moderately and mildly ill-posed problems? We have first considered the case that all the singular values of  $A$  are simple. As a key and indispensable step, we have established accurate bounds for the 2-norm distances between the underlying  $k$  dimensional Krylov subspace and the  $k$  dimensional dominant right singular subspace for the three kinds of ill-posed problems under consideration. Then we have provided other absolutely necessary background and ingredients. Based on them, we have proved that, for severely or moderately ill-posed problems with  $\rho > 1$  or  $\alpha > 1$  suitably, LSQR has the full regularization. Precisely, for  $k \leq k_0$  we have proved that a  $k$ -step Lanczos bidiagonalization produces a near best rank  $k$  approximation of  $A$  and the  $k$  Ritz values approximate the first  $k$  large singular values of  $A$  in natural order, and no small Ritz value smaller than  $\sigma_{k_0+1}$  appears before LSQR captures all the needed dominant SVD components, so that the noise  $e$  in  $b$  cannot deteriorate regularized solutions until a

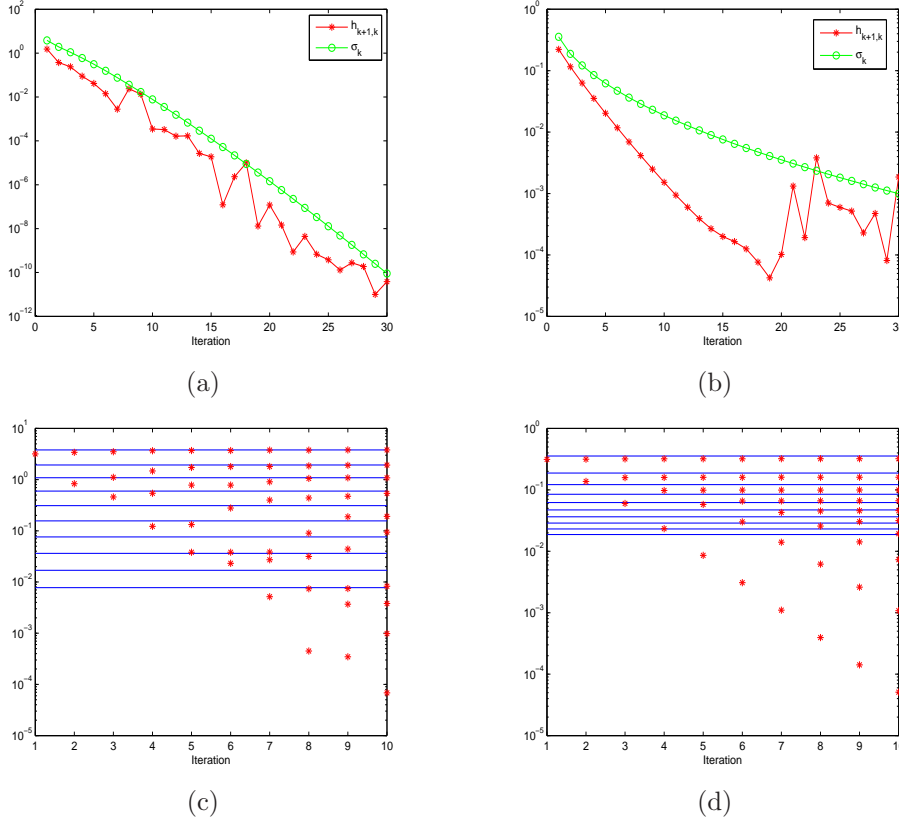


FIG. 14. (a)-(b): Decay curves of the sequences  $h_{k+1,k}$  and  $\sigma_{k+1}$ ; (c)-(d): The singular values (star) of  $\bar{H}_k$  and the ones (solid line) of  $A$  for iLaplace (left) and heat (right).

best possible regularized solution has been found. We have shown that LSQR resembles the TSVD method for these two kinds of problems. For mildly ill-posed problems, we have proved that LSQR generally has only the partial regularization since a small Ritz value generally appears before all the needed dominant SVD components are captured. Since CGLS is mathematically equivalent to LSQR, our assertions on the full or partial regularization of LSQR apply to CGLS as well.

We have derived bounds for the diagonals and subdiagonals of bidiagonal matrices generated by Lanczos bidiagonalization. Particularly, we have proved that they decay as fast as the singular values of  $A$  for severely ill-posed problems or moderately ill-posed problems with  $\rho > 1$  or  $\alpha > 1$  suitably and decay more slowly than the singular values of  $A$  for mildly ill-posed problems. These bounds are of theoretical and practical importance, and they can be used to identify the degree of ill-posedness without extra cost and decide the full or partial regularization of LSQR.

Based on some of the results established for LSQR, we have derived accurate estimates for the accuracy of the rank  $k$  approximations to  $A$  and  $A^T A$  that are involved in CGME and LSMR, respectively. We have analyzed the behavior of the smallest singular values of the projected matrices associated with CGME and LSMR. Using these results, we have shown that LSMR has the full regularization for severely and moderately ill-posed problems with  $\alpha > 1$  and  $\alpha > 1$  suitably, and it generally

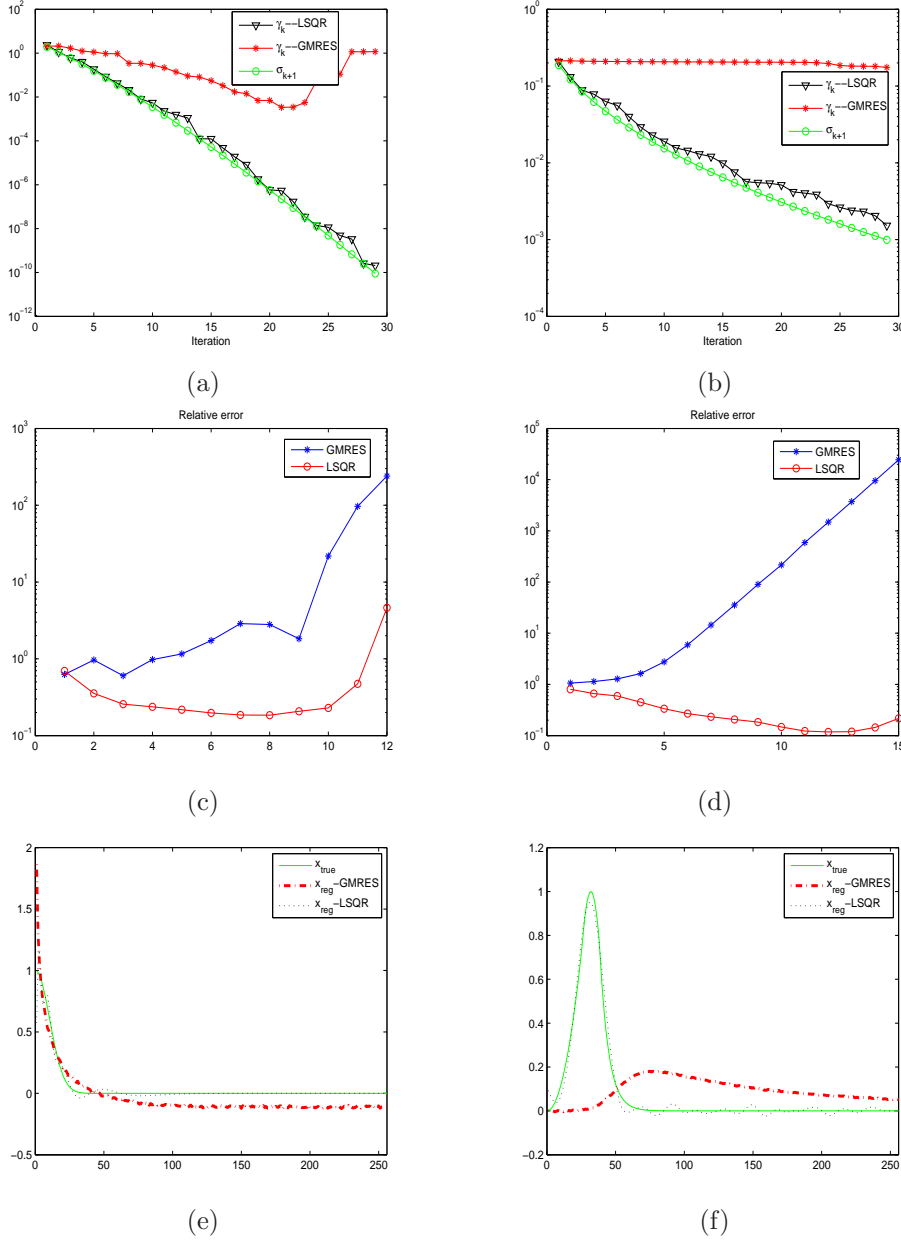


FIG. 15. (a)-(b): Decay curves of the sequences  $\gamma_k$ ,  $\gamma_k^g$ , denoted by  $\gamma_k$ -LSQR and  $\gamma_k$ -GMRES in the figure, and  $\sigma_{k+1}$ ; (c)-(d): The relative errors  $\|x^{(k)} - x_{true}\|/\|x_{true}\|$ ; (e)-(f): The regularized solutions  $x_{reg}$  obtained by LSQR and GMRES for Laplace (left) and heat (right).

has only the partial regularization for mildly ill-posed problems. In the meantime, we have shown that the regularization of CGME has indeterminacy and is inferior to LSQR and LSMR for each of three kinds of ill-posed problems. In addition, our results have indicated that the rank  $k$  approximations to  $A$  generated by Lanczos bidiagonalization are substantially more accurate than those obtained by standard

randomized algorithms [43] and the strong RRQR factorizations [42].

With a number of nontrivial modifications and reformulations, we have shown how to extend all the results obtained for LSQR, CGME and LSMR to the case that  $A$  has multiple singular values.

We have made detailed and illuminating numerical experiments and confirmed our theory on LSQR. We have also compared LSQR with GMRES and RRGMR, showing that the latter two methods do not general regularizing effects and fail to deliver regularized solutions for general nonsymmetric ill-posed problems. Theoretically, this is due to the fact that GMRES and RRGMR may work and have regularizing effects only for (nearly) symmetric or, more generally, (nearly) normal ill-posed problems, for which the left and right singular vectors are (nearly) identical to the eigenvectors of  $A$ .

Our analysis approach can be adapted to MR-II for symmetric ill-posed problems, and similar results and assertions are expected for three kinds of symmetric ill-posed problems. Using a similar approach to that in [64], the authors [65] has made an initial regularization analysis on MR-II and derived the corresponding  $\sin \Theta$  bounds, which are too large overestimates. Our approach are applicable to the preconditioned CGLS (PCGLS) and LSQR (PLSQR) [53, 56] by exploiting the transformation technique originally proposed in [12, 25] and advocated in [44, 48, 54] or the preconditioned MR-II [56, 57], all of which correspond to a general-form Tikhonov regularization involving the matrix pair  $\{A, L\}$ , in which the regularization term  $\|x\|^2$  is replaced by  $\|Lx\|^2$  with some  $p \times n$  matrix  $L \neq I$ . It should also be applicable to the mathematically equivalent LSQR variant [77] that is based on a joint bidiagonalization of the matrix pair  $\{A, L\}$  that corresponds to the above general-form Tikhonov regularization. In this setting, the Generalized SVD (GSVD) of  $\{A, L\}$  or the mathematically equivalent SVD of  $AL_A^\dagger$  will replace the SVD of  $A$  to play a central role in analysis, where  $L_A^\dagger = (I - (A(I - L^\dagger L)^\dagger A))^\dagger L^\dagger$  is call the *A-weighted generalized inverse of L* and  $L_A^\dagger = L^{-1}$  if  $L$  is square and invertible; see [53, p.38-40,137-38] and [56, p.177-183].

Finally, we highlight on hybrid Krylov iterative solvers and make some remarks, which deserve particular and enough attention in our opinion. Because of lack of a complete regularized theory on LSQR, in order to find a best possible regularized solution for a given (1.1), one has commonly been using some hybrid LSQR variants without considering the degree of ill-posedness of (1.1); see, e.g., [1, 53, 56] and the related papers mentioned in the introduction. The hybrid CGME [47] and CGLS [1, 56] have also been used. However, Björck [13] has addressed that the hybrid LSQR variants are mathematically complicated, and pointed out that it is hard to find reasonable regularization parameters and tell when to stop them reliably.

For a hybrid LSQR variant, or more generally, for any hybrid Krylov solver that first projects and then regularizes [53, 56], the situation is more serious than what has been realized. It has long commonly accepted that the approach of "*first-regularize-then-project*" is equivalent to the approach of "*first-project-then-regularize*" and they produce the same solution; see Section 6.4 and Figure 6.10 of [56]. This equivalence seems natural. Unfortunately, they are *not* equivalent when solving (1.1). Their equivalence requires the assumption that the same regularization parameter  $\lambda$  in Tikhonov regularization is *used*, so that both of them solve the same problem and compute the same regularized solution. However, as far as regularization methods are concerned, the fundamental point is that each of the two approaches *must determine* its own optimal regularization parameter  $\lambda$  which is *unknown* in advance. Mathematically, for the approach of "*first-regularize-then-project*", there is an optimal  $\lambda$  since (1.1)

satisfies the Picard condition, though its determination is generally costly and may not be computationally viable for a large (1.1). On the contrary, for the approach of "first-project-then-regularize", one must determine its optimal  $\lambda$  for each projected problem, so one will have a sequence of optimal  $\lambda$ 's. Whether or not they converge to the optimal regularization parameter of (1.3) is unclear and lacks theoretical evidence. For discrete regularization parameters in the TSVD method for (1.1) and each of the projected problems, the situation is similar. Unfortunately, for projected problems, their optimal regularization parameters and their determination may encounter insurmountable mathematical and numerical difficulties, as we will clarify below.

As is well known, the Picard condition is an absolutely necessary condition for the existence of the squares integrable solution to a linear compact operator equation; without it, regularization would be out of the question; see, e.g., [27, 81, 89]. This is also true for the discrete linear ill-posed problem, where the discrete Picard condition means that  $\|x_{true}\| \leq C$  uniformly with some (not large) constant  $C$  such that regularization is useful to compute a meaningful approximation to it [53, 56]. Nevertheless, to the best of our knowledge, the discrete Picard conditions for projected problems arising from LSQR or any other Krylov iterative solver have been paid little attention until very recently [33]. Unfortunately, a fatal problem is that *the discrete Picard conditions are not necessarily satisfied for the projected problems*. In [33], taking  $e = \mathbf{0}$ , i.e.,  $b = \hat{b}$  noise free, the authors have proved that the discrete Picard conditions are satisfied or inherited for the projected problems under the *absolutely necessary assumption* that the  $k$  Ritz values, i.e., the singular values of the projected matrix at iteration  $k$ , approximate the  $k$  large singular values of  $A$  in natural order, regularization makes sense and can be used to solve the projected problems. However, as have been stated in [53, 56] and highlighted in this paper, under such assumption, Krylov solvers themselves will find best possible regularized solutions at semi-convergence, and there is no need to continue iterating and regularize the projected problems at all, that is, no hybrid variant is needed. On the other hand, if the  $k$  Ritz values do not approximate the  $k$  large singular values of  $A$  in natural order and at least one Ritz value smaller than  $\sigma_{k_0+1}$  appears before  $k \leq k_0$ , the discrete Picard conditions are *essentially not satisfied any longer* for the projected problems starting from such  $k$  onwards. If so, regularization applied to projected problems is mathematically groundless and numerically may lead to unavoidable failure.

We take LSQR as an example for a precise statement on the discrete Picard conditions for projected problems. Recall that, in the projected problem (2.5), the noisy right-hand side is  $\|b\|e_1^{(k+1)} = P_{k+1}^T b$  with  $b = \hat{b} + e$  and the noise-free right-hand side is  $P_{k+1}^T \hat{b}$ . Then for  $k = 1, 2, \dots, n-1$  and for  $n$  arbitrarily large and  $\sigma_n \rightarrow 0$  (cf. [33]), the discrete Picard conditions for the projected problems are

$$\sup_{k,n} \|B_k^\dagger P_{k+1}^T \hat{b}\| \leq C$$

uniformly with some constant  $C$ . Numerically, for a given  $n$  and  $\sigma_n$  close to zero arbitrarily, once  $\|B_k^\dagger P_{k+1}^T \hat{b}\|$  is very large for some  $k$ , then the discrete Picard condition actually fails for the corresponding projected problem. In this case, for the projected problem, it is hard to apply regularization to the projected problem and speak of its optimal regularization parameter, which does not exist at all in the extreme case that  $\|B_k^\dagger P_{k+1}^T \hat{b}\|$  is infinitely unbounded, which amounts to stating that  $B_k$  has a singular value close to zero arbitrarily. As a result, any regularization applied to it works poorly. Indeed, for `phillips` and `deriv2` of order  $n = 1,024$  and  $10,240$ , we have observed that the hybrid LSQR exhibits considerable *erratic* other than smooth



curves of the errors between the regularized solutions and  $x_{true}$  in the dampening and stabilizing stage, causing that the hybrid LSQR is unreliable to obtain a best regularized solution; see Figure 16. Actually, the regularized solutions obtained by the hybrid LSQR after its stabilization are considerably less accurate than those by the pure LSQR itself. For *deriv2* of order  $n = 1,024$ , similar phenomena have also been observed for the hybrid MINRES and MR-II [65].

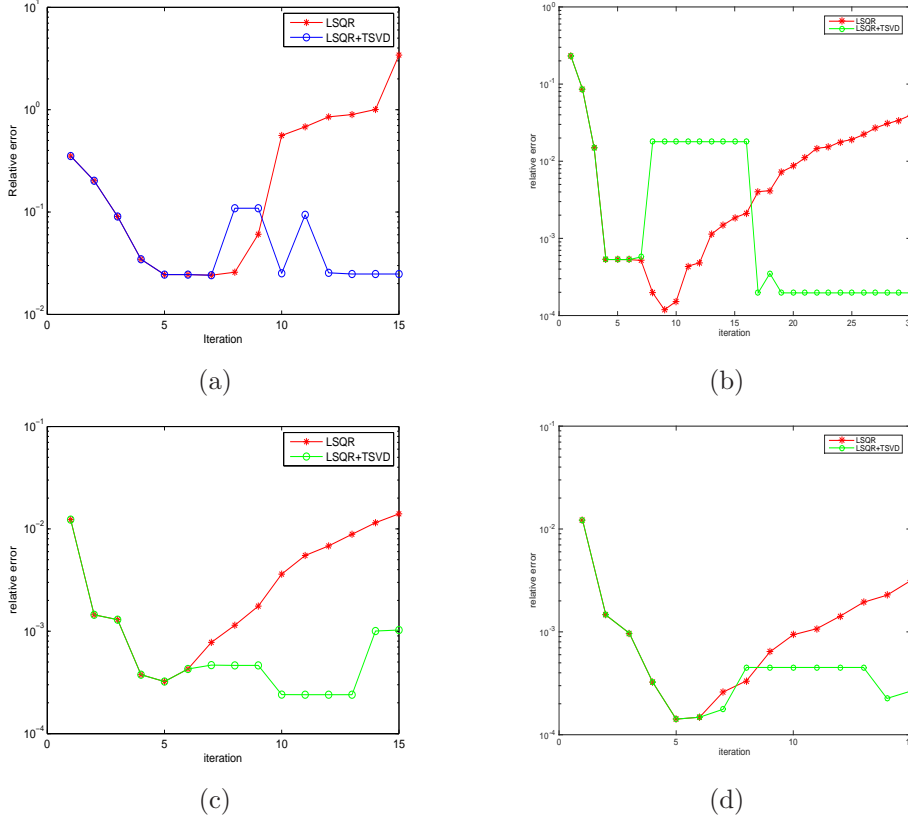


FIG. 16. (a)-(b): The relative errors  $\|x^{(k)} - x_{true}\|/\|x_{true}\|$  by LSQR and the hybrid LSQR for *phillips* of  $n = 1,024$  and  $10,240$  with  $\varepsilon = 10^{-3}$  and  $10^{-4}$ ; (c)-(d): The relative errors  $\|x^{(k)} - x_{true}\|/\|x_{true}\|$  by LSQR and the hybrid LSQR for *deriv2* of  $n = 1,024$  and  $10,240$  with  $\varepsilon = 10^{-3}$ .

The above phenomena are exactly due to the actual failure of the discrete Picard conditions for the projected problems because each of the projected matrices starts to have at least one singular value *considerably* smaller than  $\sigma_{k_0+1}$  from some iteration  $k \leq k_0$  onwards, which and whose corresponding (left and right) Ritz vectors does not approximate any singular triplet of  $A$  well. A consequence of such actual failure is that it is hard to reliably stop the hybrid variants at right iteration in order to ultimately find a best regularized solution. Therefore, for the mildly ill-posed problems and moderately ill-posed problems with  $\alpha > 1$  not enough, it is appealing to seek other mathematically solid and computationally viable variants of LSQR, LSMR and MR-II so that best possible regularized solutions can be found.

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